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Article (Published Version)

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B. J. Dalton,[1,2] Stephen M. Barnett,[3] and B. M. Garraway[1]
[1]*Sussex Centre for Optical and Atomic Physics, University of Sussex, Brighton BN1 9QH, United Kingdom*
[2]*Department of Physics, University of Queensland, St Lucia, Queensland 4072, Australia*
[3]*Department of Physics and Applied Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom*
(Received 22 February 2001; published 12 October 2001)

This paper deals with non-Markovian behavior in atomic systems coupled to a structured reservoir of quantum electromagnetic field modes, with particular relevance to atoms interacting with the field in high-Q cavities or photonic band-gap materials. In cases such as the former, we show that the pseudomode theory for single-quantum reservoir excitations can be obtained by applying the Fano diagonalization method to a system in which the atomic transitions are coupled to a discrete set of (cavity) quasimodes, which in turn are coupled to a continuum set of (external) quasimodes with slowly varying coupling constants and continuum mode density. Each pseudomode can be identified with a discrete quasimode, which gives structure to the actual reservoir of true modes via the expressions for the equivalent atom-true mode coupling constants. The quasimode theory enables cases of multiple excitation of the reservoir to now be treated via Markovian master equations for the atom-discrete quasimode system. Applications of the theory to one, two, and many discrete quasimodes are made. For a simple photonic band-gap model, where the reservoir structure is associated with the true mode density rather than the coupling constants, the single quantum excitation case appears to be equivalent to a case with two discrete quasimodes.

DOI: 10.1103/PhysRevA.64.053813 PACS number(s): 42.50.Lc, 42.70.Qs

I. INTRODUCTION

The quantum behavior of a small system coupled to a large one has been the subject of many studies since quantum theory was first formulated. The small system is usually of primary interest and generally microscopic (atom, nucleus, molecule, or small collections of these) but currently systems of a more macroscopic nature (Bose condensate, superconductor, quantum computer) are being studied. The large system is invariably macroscopic in nature (free space or universe modes of the electromagnetic (EM) field, lattice modes in a solid, collider atoms in a gas) and is of less interest in its own right, being primarily of relevance as a reservoir or bath affecting the small system in terms of relaxation and noise processes. The large system is often a model for the entire external environment surrounding the small system. Changes in the small system states (described in terms of its density operator) can be divided into two sorts—effects on the state populations (energy loss or gain) or effects on the state coherences (decoherence or induced coherence). Equivalently, quantum information (described via the von Neumann entropy) would be lost or gained due to the interaction with the environment, and its loss is generally associated with decoherence. Interestingly, as the small system becomes larger or occupies states that are more classical the time scale for decoherence can become much smaller than that for energy loss. This is of special interest in quantum information processing [1–3] where the small system is a collection of qbits making up a quantum computer weakly coupled to the outside world, or in measurement theory [4–7], where the small system is a microsystem being measured, coupled to an apparatus (or pointer) that registers the results. For quantum computers it is desirable that decoherence is negligible during the overall computation time [8] (otherwise error correction methods have to be incorporated, and this is costly in terms of processing time) whereas in measurement theory, environment induced decoherence [4,9] is responsible for the density operator becoming diagonal in the pointer basis (otherwise a macroscopic superposition of pointer readings would result).

A standard method for describing the reservoir effects on the small system is based on the Born-Markoff master equation for the system density operator [10–13]. This depends on the correlation time for the reservoir (as determined from the behavior of two-time correlation functions for pairs of reservoir operators involved in the system-reservoir interaction) being very short compared to that of the relaxation and noise processes of the system. In general terms, the more slowly varying the coupling constants for this interaction or the density of reservoir states are with reservoir frequencies, the shorter the correlation time will be. For many situations in the field of quantum optics, nuclear magnetic resonance (NMR), and solid-state physics, the Born-Markoff master equation provided an accurate description of the physics for the system. Elaborations or variants of the method such as quantum state trajectories [14,15], Fokker-Planck or c-number Langevin equations [10,16], and quantum Langevin equations [10,11,13] are also used. Sometimes an apparently non-Markovian problem can be converted to a Markovian one by a more suitable treatment of the internal system interactions (for example, the use of dressed atom states [17,18] for treating driven atoms in narrow-band squeezed vacuum fields [19,20]).

However, situations in which the reservoir correlation times are too long for the system time scales of interest—and thus the standard Born-Markoff approach is no longer appropriate—have also been studied. An early paper on this subject is Ref. [21], where atomic decay into a narrow resonance of an optical cavity is treated. Two regimes are distinguished—a weak-coupling regime, where the atomic behavior is Markovian and irreversible decay occurs, and a

strong-coupling regime, where non-Markovian atomic dynamics occur accompanied by an oscillatory reversible decay. In such situations a structured rather than a flat reservoir situation applies, and the recent reviews in Refs. [22,23] indicate the current upsurge of interest in non-Markovian behavior as well as providing the reader with references to some of the earlier work. The situations studied include cases where the reservoir coupling constants vary significantly with frequency, such as the interaction of atom(s) or quantum dots with light in high Q cavities Refs. [21,24], including microcavities (see, for example, Refs. [25–29]) and microspheres (see, for example, Refs. [30,31]). Laser-driven atoms in structured reservoirs (resulting in modified resonance fluorescence and non-Markovian atomic dynamics) have also been treated (see for example, Refs. [32–37]). Other cases where the reservoir mode densities have structure in the form of gaps and non-analytic behavior also occur, such as an atom (or many atoms—super-radiance) interacting with light in photonic band-gap materials [22,38–42]. Non-Markovian effects in the excitation of continuum state resonances due to threshold effects have been studied in Ref. [43]. Also, quantum feedback situations [44,45] can involve significant time delays in the feedback circuit, and thus result in non-Markovian dynamics for the system itself. Furthermore, systems with several degrees of freedom, such as in quantum measurements (for example, the Stern-Gerlach experiment) could involve situations where the decoherence times associated with some degrees of freedom (such as the position of the atomic spin) could become so short that the Markoff condition might no longer be valid, and the effects of such non-Markovian relaxation on the decoherence times associated with more important degrees of freedom (atom spin states) would be of interest.

A number of methods for treating non-Markovian processes have been developed and successfully applied to problems involving structured reservoirs. Apart from direct numerical simulations (for example, Ref. [46]) these include the Zwanzig-Nakajima non-Markovian master equation and its extensions [47–49], the time-convolutionless projection operator master equation [50], Heisenberg equations of motion [40,51], stochastic wave-function methods for non-Markovian processes [52–57], methods based on the essential states approximation or resolvent operators [22,39,58], the pseudomode approach [59,60], Fano diagonalization [61,12,62] and the sudden decoherence approximation [63]. The last four methods are simple to apply, providing clear physical insight into the processes involved, and their key features follow.

The *essential states method* involves the set of coupled amplitude equations for the physically important states. This method can become complicated when multiple excitations of the reservoir are involved, since the equations become unwieldy and difficult to solve. The method of solution generally involves Laplace transform methods, the final expressions for the amplitudes are obtained via contour integration. This does have the advantage of enabling nonanalytic effects due to thresholds [43] and band gaps [39] to be treated. The *pseudomode method* starts from the essential states approximation and is based on the idea of enlarging the system to include part of the reservoir (the pseudomode—which could be bosonic or fermionic depending on the case) thereby forming a bigger system in which the Markoff approximation applies when the coupling to the remainder of the reservoir is treated. At present the pseudomode method is restricted to single reservoir excitation cases, but like the essential states approach, has the advantage of giving exact solutions without making use of perturbation theory. The pseudomodes (or rather their amplitudes) are mathematically defined in terms of the positions and residues of simple poles of the reservoir structure function in the lower-half complex-frequency plane, where the reservoir structure function is proportional to the reservoir mode density times the modulus squared of the coupling constants. Each pole is associated with a pseudomode. Since it is related to the description of the reservoir in terms of its true modes [64–66]—which are solutions of the Helmholtz equation for the exact spatially dependent permittivity that describes the optical systyem—the pseudomode theory is dependent on the reservoir structure function having simple poles in the lower-half plane, and is therefore not yet applicable to cases such as realistic photonic band-gap systems where nonanalytic behavior of the reservoir structure function occurs. Nevertheless, in other cases it can be applied without knowing why the poles occur, though the disadvantage of this is that the physical nature of the pseudomodes is then left obscure. The pseudomode theory has also been used to obtain exact Markovian master equations for the combined atom plus pseudomodes system. The *Fano diagonalization method* involves replacing the original system-reservoir Hamiltonian by a diagonal form, and relates the causes of non-Markovian effects to various underlying features displayed by the new Hamiltonian (such as the presence of bound states in the case of atom lasers). In certain cases it is closely related to the pseudomode method, as will be seen below. A combination of an improved pseudomode method with the inclusion via Fano diagonalization of a suitable model describing the physics of the reservoir, would advance the methodology for a simple treatment of non-Markovian behavior. The *sudden decoherence method* enables decoherence effects on time scales that are short compared to system Bohr periods to be treated simply by ignoring the system Hamiltonian. In certain respects this method is more universal than the others but it is restricted to short-time scales, and therefore has a limited capacity for development. It has, however, been applied to improve our understanding of short-time scale decoherence in general systems [63] .

This paper deals with the relationship between the current pseudomode method for single-quantum reservoir excitations and the Fano diagonalization method for situations where the reservoir structure is due to the presence of a discrete system of (quasi) modes, which are coupled to other continuum (quasi) modes. This important case applies to atomic systems coupled to the quantum EM field in high Q resonant cavities, such as microspheres or microcavities. The aim is to understand the physical origin of the pseudomodes in terms of quasimodes [67,68,65], which are solutions of the Helmholtz equation for an idealized spatially dependent permittivity that approximately models the actual optical system. In the

case of cavity QED, one discrete quasimode can be chosen to occur for each resonance of the cavity, though each such resonance is associated with large numbers of true modes [69,65]. A further objective of this paper is to see whether the pseudomode theory restriction to single quantum excitations of the reservoir can be lifted through the explicit introduction of this physical model for the pseudomodes. It is shown that the pseudomode method for single quantum excitations of the structured reservoir can be obtained by applying the Fano diagonalization method to a system featuring a set of discrete quasimodes [67,68,65] together with a set of continuum quasimodes, whose mode density is slowly varying. The structured reservoir of true modes [64–66] is thus replaced by the quasimodes. The interaction between the discrete and continuum quasimodes is treated in the rotating-wave approximation and assuming slowly varying coupling constants [69,70]. The atomic system is assumed to be only coupled to the discrete quasimodes. The density of continuum quasimodes is explicitly included in the model. Although the behavior of the atomic system itself is non-Markovian, the enlarged system obtained by combining the discrete quasimodes with the atomic system now exhibits Markovian dynamics. The discrete quasimodes are identified as pseudomodes. The continuum quasimodes are identified as the flat reservoir to which the enlarged Markovian system is coupled. Explicit expressions for the atom-true modes coupling constants are obtained, exhibiting the rapidly varying frequency dependence characteristic of structured reservoirs. At present the treatment is restricted to cases where threshold and band-gap effects are unimportant, but may be applicable to two-dimensional photonic band-gap materials. However, the problem of treating multiple excitation processes for certain types of structured reservoirs can now be treated via the quasimode theory, since the Markovian master equation for the atom-quasimode system applies for cases involving multilevel atoms or cases of several excited two-level atoms. Further extensions of the treatment to allow for atomic systems driven by single mode external laser fields are also possible, with the original atomic system being replaced by the dressed atom.

The plan of the paper is as follows. In Sec. II the key features of pseudomode theory are outlined. Section III presents the Fano diagonalization theory for the quasimode system, with details covered in Appendices A, B, and C. In Sec. IV specific cases such as one or two discrete quasimodes or where the variation of discrete-continuum coupling constants can be ignored, are examined, giving results for the atom-true mode coupling constants and reservoir structure functions in these situations. Section V contains the Markovian master equation for the atom plus discrete quasimode systems. Section VI briefly examines the situation where coupling constants and mode densities are not slowly varying. Conclusions and comments are set out in Sec. VII.

II. PSEUDOMODE THEORY

The simplest case to which pseudomode theory [59] can be applied is that of a two-level atom coupled to the modes of the quantum EM field—which constitutes the structured reservoir. Only one photon excitation process will occur. However, the formalism would also apply to any spin-1/2 fermion system coupled to a bath of bosonic oscillators. The Hamiltonian is given in the rotating-wave approximation by

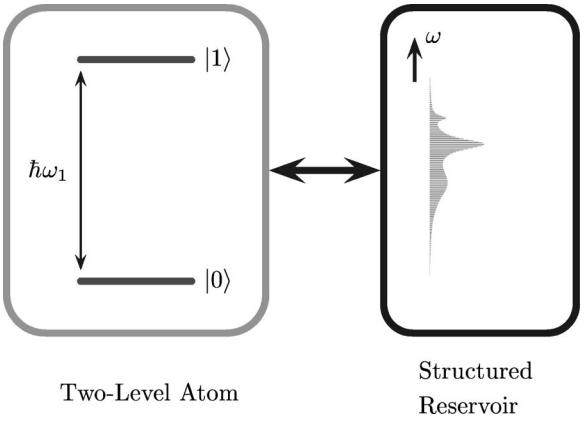

FIG. 1. Illustration of a two-level atom coupled to a structured reservoir.

$$\hat{H}=\sum_{\lambda}\hbar\omega_{\lambda}\hat{a}_{\lambda}^{\dagger}\hat{a}_{\lambda}+\frac{1}{2}\hbar\omega_1(\hat{\sigma}^{+}\hat{\sigma}^{-}-\hat{\sigma}^{-}\hat{\sigma}^{+})$$

$$+\sum_{\lambda}(\hbar g_{\lambda}^{*}\hat{a}_{\lambda}\hat{\sigma}^{+}+\text{H.c.}), \tag{1}$$

where $\hat{\sigma}^{+},\hat{\sigma}^{-}$ are the usual atomic spin operators, $\hat{a}_{\lambda}$, $\hat{a}_{\lambda}^{\dagger}$ are the annihilation creation operators for the mode λ of the field, ω_1 is the atomic transition frequency, ω_{λ} is the mode frequency, and g_{λ} are the coupling constants. This system is illustrated in Fig. 1.

To describe a one-photon excitation process, the initial condition is the atom excited and no photons present in the field. Hence the initial Schrodinger picture state vector is

$$|\Psi(0)\rangle=|1\rangle|\ldots 0_{\lambda}\ldots\rangle. \tag{2}$$

In the essential states approach, the state vector at later time t will be a superposition of the initial state and states with the atom in its lower state and one photon in various modes λ. With $\tilde{c}_1,\tilde{c}_{\lambda}$ defining the complex amplitudes for the atomic excited state and the one photon states, the state vector is

$$|\Psi(t)\rangle=\tilde{c}_1(t)\mathrm{e}^{-i\omega_1 t}|1\rangle|\ldots 0_{\lambda}\ldots\rangle$$

$$+\sum_{\lambda}\tilde{c}_{\lambda}(t)e^{-i\omega_{\lambda}t}|0\rangle|\ldots 1_{\lambda}\ldots\rangle. \tag{3}$$

Substitution into the time-dependent Schrodinger equation leads to the following coupled complex amplitude equations:

$$i\frac{d}{dt}\tilde{c}_1=\sum_{\lambda}g_{\lambda}^{*}e^{-i\Delta_{\lambda}t}\tilde{c}_{\lambda},$$

$$i\frac{d}{dt}\tilde{c}_\lambda = g_\lambda e^{i\Delta_\lambda t}\tilde{c}_1, \tag{4}$$

where $\Delta_\lambda = \omega_\lambda - \omega_1$ are detunings.

Formally eliminating the amplitudes for the one-photon states enables an integrodifferential equation for the excited atomic amplitude to be derived. This is

$$\frac{d}{dt}\tilde{c}_1(t) = -\int_0^t d\tau\, \tilde{G}(\tau)\tilde{c}_1(t-\tau) \tag{5}$$

and involves a kernel $\tilde{G}$ given by

$$\tilde{G}(\tau) = \sum_\lambda |g_\lambda|^2 e^{-i\Delta_\lambda \tau} = \int d\omega_\lambda\, \rho(\omega_\lambda)|g_\lambda|^2 e^{-i\Delta_\lambda\tau}. \tag{6}$$

The mode density $\rho(\omega_\lambda)$ is introduced after replacing the sum over λ by an integral over the mode angular frequency ω_λ.

It is apparent from Eq. (5) that the behavior of the atomic system only depends on the reservoir structure function $D(\omega_\lambda)$ for this single-quantum excitation case defined by

$$\rho_\lambda |g_\lambda|^2 = \frac{\Omega^2}{2\pi} D(\omega_\lambda), \tag{7}$$

where a transition strength Ω is introduced to normalize D so that its integral gives 2π. The transition strength Ω is given by

$$\Omega^2 = \int d\omega_\lambda\, \rho(\omega_\lambda)|g_\lambda|^2. \tag{8}$$

The reservoir structure function $D(\omega_\lambda)$ enables us to describe the various types of reservoir to which the atomic system is coupled. If D is slowly varying as a function of ω_λ then the reservoir is ''flat,'' while ''structured'' reservoirs are where D varies more rapidly, as seen in Fig. 1. There are of course two factors involved in determining the behavior of D—the mode density $\rho(\omega_\lambda)$ and the coupling constant via $|g_\lambda|^2$. Either or both can determine how structured the reservoir is. Photonic band-gap materials are characterized by mode densities that are actually zero over the gaps in the allowed mode frequencies, and which have nonanalytic behaviors near the edges of the band gaps. All mode densities are zero for negative ω_λ, so threshold effects are possible — see Ref. [43], for example. In cavity QED situations, such as for microspheres and other high Q cavities, the coupling constant varies significantly near the cavity resonant frequencies, so in these cases it is the coupling constant that gives structure to the reservoir. For the present it will be assumed that (apart from simple poles) D is analytic in the lower-half complex ω_λ plane, and any other nonanalytic features can be disregarded. It is recognized of course that this restriction places a limit on the range of applicability of the theory, though it may be possible to extend this range by representing the actual function $D(\omega_\lambda)$ in an approximate form that satisfies the analyticity requirements. In addition (in order to calculate the contour integrals) it will be assumed that D tends to zero at least as fast as $1/|\omega_\lambda|$ as $|\omega_\lambda|$ tends to infinity.

Based on the above assumption regarding the reservoir structure function D, the kernel G may be evaluated in terms of the poles and residues of $D(\omega_\lambda)$ in the lower-half complex ω_λ plane. It is assumed that these simple poles can be enumerated. The poles are located at $z_1, z_2, \ldots z_l \ldots$ and their residues are $r_1, r_2, \ldots r_l \ldots$. The pole z_l may be expressed in terms of a real angular frequency ω_l and a width factor Γ_l via $z_l = \omega_l - i\Gamma_l/2$. Contour integration methods show that the sum of the residues equals i. The kernel is obtained in the form

$$\tilde{G}(\tau) = -i\Omega^2 \sum_l r_l e^{-i(z_l-\omega_1)\tau}. \tag{9}$$

The integrodifferential equation (5) for the excited atomic amplitude involves a convolution integral on the right-hand side and may be solved using Laplace transform methods. The atomic behavior obtained is well known [21,64] and will not be rederived here. It is found that there are two regimes, depending on the ratio of the transition strength to typical width factors. These are (a) a strong-coupling regime with non-Markovian atomic dynamics, which occurs when $\Omega \gg \Gamma$, and (b) a weak-coupling regime with Markovian atomic dynamics, occuring when $\Omega \ll \Gamma$.

The pseudomode approach continues by considering poles of the reservoir structure function $D(\omega_\lambda)$ in the lower-half complex ω_λ plane. Each pole will be associated with one pseudomode. Reverting to Schrodinger picture amplitudes via $c_1(t) = \tilde{c}_1(t)\mathrm{e}^{-i\omega_1 t}$ etc., pseudomode amplitudes associated with each pole of D are introduced as defined by

$$b_l(t) = -i\Omega\sqrt{-ir_l}\, e^{-iz_l t}\int_0^t dt'\, e^{iz_l t'} c_1(t'). \tag{10}$$

From the definition of b_l and by substituting the form [Eq.(9)] for the kernel G that involves the poles of D, it is not difficult to show that the excited atomic amplitude and the pseudomode amplitudes satisfy the following coupled equations:

$$i\frac{dc_1(t)}{dt} = \omega_1 c_1(t) + \sum_l \mathcal{K}_l b_l(t),$$

$$i\frac{db_l(t)}{dt} = z_l b_l(t) + \mathcal{K}_l c_1(t), \tag{11}$$

where $\mathcal{K}_l = \Omega\sqrt{-ir_l}$ are pseudomode coupling constants. In general, the residues r_l are not pure imaginary, so the pseudomode coupling constants are not real.

The important point is that the atom plus pseudomodes system now satisfies Markovian equations [Eq.(11)]. With a finite (or countable) set of pseudomodes, the original atom plus structured continuum has now been replaced by a simpler system, which still enables an exact description of the

atomic behavior to be obtained. *Exact* master equations involving the pseudomodes have been derived, and in general the pseudomodes can be coupled (see Ref. [59]). There are however, difficulties in cases where the pseudomode coupling constants are not real, which can occur in certain cases where there are several pseudomodes. Apart from the general difficulty associated with situations where (apart from having simple poles) the reservoir structure function D is not analytic in the lower-half complex plane, there is also considerable difficulty in extending the above theory to treat cases where multiple excitations of the structured reservoir occur, such as when the two-level atom is replaced by a three-level atom in a cascade configuration with the atom initially in the topmost state. The problem is that applying the usual essential states approach leads to two (or more) photon states now appearing in the state vector [cf. Eq.(3)], and the resulting coupled amplitude equations [cf. Eq.(4)] do not apear to facilitate the sucessive formal elimination of the one, two, . . . photon amplitudes, as is possible in the single-photon excitation case treated above. It is, therefore, not clear how pseudomode amplitudes can be introduced, along the lines of Eq. (10), so the pseudomode method has not yet been generalized from its original formulation to allow for multiple reservoir excitations.

III. FANO DIAGONALIZATION FOR A QUASIMODE SYSTEM

A. Description of the approach

The case of multiple excitation of a structured reservoir involves systems more complex than the two-level atom treated above. It will be sufficient for the purpose of linking the pseudomode and Fano diagonalization methods to consider single multilevel atomic systems, although multiatom systems would also be suitable as both systems could result in multiphoton excitations of the quantum EM field. Accordingly the two-level Hamiltonian given as the second term in Eq. (1) is now replaced by the multilevel atomic Hamiltonian:

$$\hat{H}_A = \sum_k \eta_k \hbar \omega_k (\hat{\sigma}_k^+ \hat{\sigma}_k^- - \hat{\sigma}_k^- \hat{\sigma}_k^+). \tag{12}$$

The index k represents an atomic transition associated with a pair of energy levels ($k \equiv \{u,l\}$) with energy difference $\hbar\omega_k$. The quantities η_k are numbers chosen so that $\hat{H}_A$ equals the atomic Hamiltonian, apart from an additive constant energy; for example, in a two-level atom $\eta = \frac{1}{2}$ for the single transition, while in a three-level atom in a V configuration with degenerate upper levels $\eta_1 = \eta_2 = \frac{1}{3}$ for the two optical frequency transitions, and $\eta_3 = 0$ for the zero frequency transition. Details are set out in Appendix A. The atomic transition operators are $\hat{\sigma}_k^+ \equiv |u\rangle\langle l| \equiv (\hat{\sigma}_k^-)^\dagger$. As the Hamiltonians for other fermionic systems can also be written in the same form as in Eq. (12), the treatment is not just restricted to single multilevel atom systems. The case of an atom driven by a single mode laser field can also be treated. Here the atomic Hamiltonian would be replaced by the sum of the atomic Hamitonian, the Hamiltonian for the single laser mode, and the atom-laser mode coupling term. In effect the atomic Hamitonian is replaced by the dressed atom Hamiltonian [71].

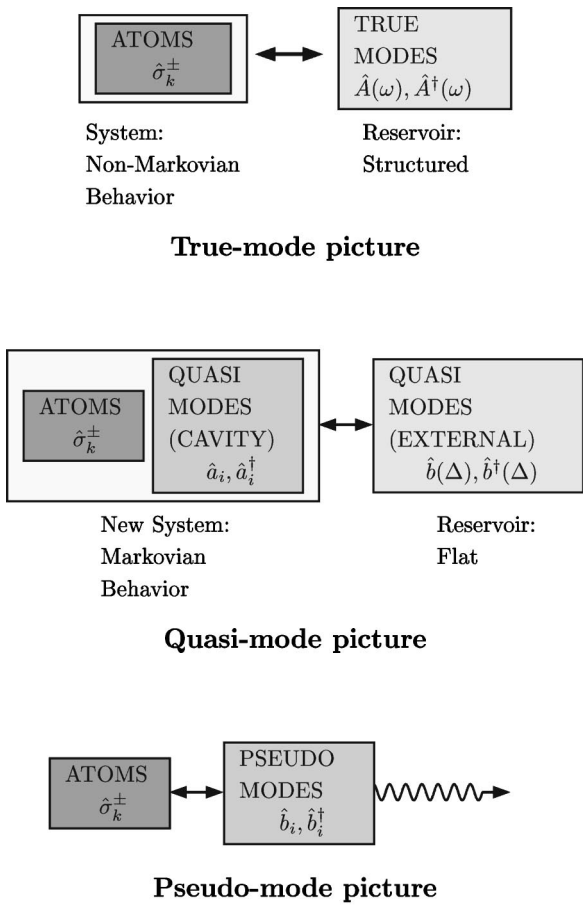

FIG. 2. Three pictures of the coupled atomic system. In the *true mode picture*, the atom is coupled directly to true modes that have structure. In the *quasimode picture* the atoms are coupled to quasimodes, which are in turn coupled to external quasimodes. In the *pseudomode picture* the atoms are coupled to dissipative pseudomodes.

As indicated in Sec. II, an important pseudomode situation is where the reservoir structure is due to the presence of a discrete system of (quasi) modes, which are coupled to other continuum (quasi) modes with slowly varying coupling constants. This important case applies to atomic systems coupled to the quantum EM field in high Q resonant cavities, such as microspheres or microcavities. The Fano diagonalization method is then based around the idea that the structured reservoir of the quantum EM field modes can be described in two different ways, which will now be outlined. Figure 2 illustrates these two descriptions, along with that involving pseudomodes.

1. Quasi modes

The first approach is to treat the quantum EM field in terms of a quasimode description [67,68,65]. The quasimode functions are here obtained as solutions of the Helmholtz

equation for an idealized spatially dependent permittivity that approximately models the actual optical system. They are not Fox-Li modes [72], which are obtained by a different principle as eigenfunctions of a non-Hermitian operator constructed via applying the paraxial approximation to the Huygen-Fresnel integral [73]. Such non-Hermitian mode functions and their adjoint modes satisfy biorthogonality relations, unlike the normal orthogonality relations satisfied by both true modes and quasimodes. The quasimodes behave as coupled quantum harmonic oscillators. These consist of two types; the first is a set of discrete quasimodes, the second is a set of continuum quasimodes. In a typical structured reservoir situation for the area of cavity QED [69], the quasimodes represent a realistic description of the physical system. The discrete modes are cavity quasimodes—one for each cavity resonance and appropriate for describing the EM field inside the cavity and the continuum modes are external quasimodes that describe the field outside the cavity. The interaction between the discrete and continuum quasimodes will be treated in the rotating-wave approximation assuming slowly varying coupling constants [69,68,70]. Rotating-wave approximation couplings between the discrete quasimodes are also included, but couplings between the continuum quasimodes are not included—such couplings can be removed by pre-diagonalization. For the quasimode description the field Hamiltonian is given by

$$\hat{H}_F = \sum_i \hbar\omega_i \hat{a}_i^\dagger \hat{a}_i + \sum_{i\neq j} \hbar v_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_i \int d\Delta\, \rho_c(\Delta)[\hbar W_i(\Delta)\hat{a}_i^\dagger \hat{b}(\Delta) + \text{H.c.}] + \int d\Delta\, \rho_c(\Delta)\, \hbar\Delta \hat{b}^\dagger(\Delta)\hat{b}(\Delta), \tag{13}$$

where $\hat{a}_i$, $\hat{a}_i^\dagger$ are the annihilation creation operators for the discrete quasimode i, ω_i is its frequency, $\hat{b}(\Delta), \hat{b}^\dagger(\Delta)$ are the annihilation creation operators for the continuum quasimode of frequency Δ, the coupling constants between the i,j discrete quasimodes are v_{ij} $(v_{ij}=v_{ji}^*)$, while the quantity $W_i(\Delta)$ is the coupling constant between the i discrete and Δ continuum quasimodes. The integrals over the quasicontinuum frequency Δ involve a quasicontinuum mode density $\rho_c(\Delta)$. Both $W_i(\Delta)$ and $\rho_c(\Delta)$ are usually slowly varying. The discrete quasimode annihilation creation operators satisfy Kronecker delta commutation rules, while those for the continuum quasimode operators satisfy Dirac delta function commutation rules:

$$[\hat{a}_i, a_j^\dagger] = \delta_{ij},$$

$$[\hat{b}(\Delta), \hat{b}^\dagger(\Delta')] = \delta(\Delta - \Delta')/\rho_c(\Delta). \tag{14}$$

The ρ_c factor on the right-hand side gives annihilation and creation operators that are dimensionless.

For the quasimode description the interaction between the atomic system and the quantum EM field will be given in the rotating-wave approximation and only involve coupling to the discrete quasimodes. This would apply for the typical structured reservoir situation for the area of cavity QED in the familiar case where the atoms are located inside the cavity. The energy of an excited atom escapes to the external region in a two-step process: first, a photon is created in a discrete (cavity) quasimode via the atom-discrete quasimode interaction, second, this photon is destroyed and a photon is created in a continuum (external) quasimode via the discrete-continuum quasimode coupling. For the quasimode description, the atom-field interaction will be given as

$$\hat{H}_{AF} = \sum_k \sum_i (\hbar\lambda_{ki}^* \hat{a}_i \hat{\sigma}_k^+ + \text{H.c.}), \tag{15}$$

where λ_{ki} is the coupling constant for the k atomic transition and the i quasimode.

2. True modes

The second way of describing the quantum EM field is in terms of its true modes [64–66]. The true mode functions are here obtained as solutions of the Helmholtz equation for the actual spatially dependent permittivity that applies to the optical system. The true modes behave as uncoupled quantum harmonic oscillators. These modes are also used in cavity QED and are often referred to as ''universe modes.'' The pseudomode theory presented in Sec. II is also based on true modes. For frequencies near the cavity resonances, these modes are large inside the cavity and small outside; for frequencies far away from the resonance, the opposite applies. The distinction between true modes and quasimodes is discussed in some detail in recent papers [67,74] and their detailed forms and features in the specific case of a planar Fabry-Perot cavity are demonstrated in Ref. [69]. In terms of true modes, the field Hamiltonian is now given in the alternative form as

$$\hat{H}_F = \int d\omega\, \rho(\omega)\hbar\omega \hat{A}^\dagger(\omega)\hat{A}(\omega), \tag{16}$$

where $\hat{A}(\omega)$, $\hat{A}^\dagger(\omega)$ are the annihilation creation operators for the continuum true mode of frequency ω. The integrals over the quasicontinuum frequency ω involve the true continuum mode density $\rho(\omega)$, which is not in general the same function as $\rho_c(\Delta)$. It is also not necessarily a slowly varying function of ω. The continuum true mode annihilation creation operators satisfy Dirac delta function commutation rules:

$$[\hat{A}(\omega), \hat{A}^\dagger(\omega')] = \delta(\omega - \omega')/\rho(\omega). \tag{17}$$

In all these Hamiltonians the coupling constants have dimensions of frequency, while the annihilation and creation operators are dimensionless, as are the atomic transition operators.

3. Relating quasi and true modes

As will be demonstrated in Sec. III B, Fano diagonalization involves determining the relationship between the true mode annihilation operators $\hat{A}(\omega)$ and the quasimode anni-

hilation operators $\hat{a}_i$ and $\hat{b}(\Delta)$. The $\hat{A}(\omega)$ will be written as a linear combination of the $\hat{a}_i$ (sum over i) and $\hat{b}(\Delta)$ (integral over Δ) [see Eq. (22) below], which involves the functions $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$. This relationship can be inverted to give the $\hat{a}_i$ as an integral over ω of the $\hat{A}(\omega)$ [see Eq. (52) below]. This enables the true mode form of the atom-field interaction to be given as

$$\hat{H}_{AF}=\sum_k \sum_i \int d\omega\, \rho(\omega)[\hbar\lambda_{ki}^{*}\alpha_i^{*}(\omega)\hat{A}(\omega)\hat{\sigma}_k^{+}+\text{H.c.}]. \tag{18}$$

Comparing Eqs. (15) and (18) we see that the atom-true mode coupling constant $g^k(\omega)$ (for the k atomic transition and the ω true mode) is given by the expression

$$g^k(\omega)=\sum_i \lambda_{ki}\alpha_i(\omega). \tag{19}$$

This can be a complicated function of ω in a structured reservoir, as will be seen from the forms obtained for the function $\alpha_i(\omega)$ [for example, Eq. (67)]. This expression for the atom-true mode coupling constant is one of the key results in our theory, and enables the pseudomode and quasimode descriptions of decay processes for structured reservoirs to be related. Note that the true mode coupling constant now involves two factors: the atom-quasimode coupling constant λ_{ki}, and the function $\alpha_i(\omega)$ that arises from the Fano diagonalization process.

For the situation where only a single atomic transition k is involved, the equivalent reservoir structure function is given by

$$D^k(\omega)=C\rho(\omega)|g^k(\omega)|^2, \tag{20}$$

where C is the normalizing constant, which for convenience we will set equal to unity as it does not contain any ω dependence. This expression will be used to compare the results from the quasimode approach to those of the present single quantum excitation pseudomode theory. As we will see, the true mode density cancels out.

Finally, athough our results are still correct for cases where the quasimode density $\rho_c(\Delta)$ and the coupling constants $W_i(\Delta)$ are not restricted to being slowly varying functions of Δ, their utility, where this is not the case, is somewhat limited. The theory is mainly intended to apply to the important pseudomode situation, where the reservoir structure is actually due to the presence of a discrete system of quasimodes that are coupled to other continuum quasimodes via slowly varying coupling constants. For example, the quantum EM field in high Q resonant cavities can be accurately described in terms of the quasimode model that has these features, the discrete quasimodes being the cavity quasimodes (linked to the cavity resonances) with which the atoms inside the cavity interact, and the continuum quasimodes being the external modes.

As pointed out previously, the structured reservoir can be any set of bosonic oscillators, not just the quantum EM field. The above treatment would thus apply more generally, and we would then refer to discrete quasioscillators, continuum quasioscillators, or true oscillators. The physical basis for a quasimode description of the reservoir of bosonic oscillators will depend on the particular situation; in general they will be idealized approximate versions of the true modes.

B. Diagonalization of the quasimode Hamiltonian: Dressing the quasimode operators

1. Basic equations for Fano diagonalization

We start with a multiple quasimode description of the quantum EM field, for which the Hamiltonian is given above as Eq. (13). This Hamiltonian can also be written in terms of the true mode description as in Eq. (16), and the problem is to relate the true mode annihilation operators $\hat{A}(\omega)$ in terms of the quasimode annihilation operators $\hat{a}_i$ and $\hat{b}(\Delta)$. In view of the rotating-wave approximation form of the Hamiltonian, the quasimode creation operators are not involved in the relationship [67]. Fano diagonalization for the nonrotating wave approximation has been treated for the case of a single mode coupled to a reservoir in Refs. [75,76]. In making a Fano diagonalization, we will follow the lines of Ref. [12] (Sec. 6.6 on dressed operators), rather than Ref. [62], but note that a new feature here is the presence of the mode-mode coupling term in the Hamiltonian Eq. (13). In addition, we explicitly include the mode densities from the beginning. The physical realization of the quasimode model for the EM field really determines the quasicontinuum mode density $\rho_c(\Delta)$, just as it does the coupling constants $v_{ij}, W_i(\Delta)$, and λ_{ki}. It is therefore important to be able to find the $\rho_c(\omega)$ dependence of quantities such as the reservoir structure function $D(\omega)$ [as we will see, the final expression [Eq. (50)] for the latter does not involve the true mode density $\rho(\omega)$]. It is of course possible to scale all the other quantities to make $\rho=\rho_c=1$, and then rescale afterwards to allow for the actual ρ,ρ_c that apply for the system of interest, but this would lead to a great deal of duplication of the results we present. For completeness, the scaling is set out in Appendix B.

From the form of the true mode Hamiltonian in Eq. (16) and the commutation rules Eq. (17) to be satisfied by the $\hat{A}(\omega)$, it is clear that the true mode annihilation operators are eigenoperators of the quantum field Hamiltonian $\hat{H}_F$ and must satisfy

$$[\hat{A}(\omega),\hat{H}_F]=\hbar\omega\hat{A}(\omega). \tag{21}$$

In general, the true mode annihilation operators $\hat{A}(\omega)$ can be expressed as linear combinations of the quasimode annihilation operators $\hat{a}_i$ and $\hat{b}(\Delta)$ in the form [68,67]

$$\hat{A}(\omega)=\sum_i \alpha_i(\omega)\hat{a}_i+\int d\Delta\, \rho_c(\Delta)\beta(\omega,\Delta)\hat{b}(\Delta), \tag{22}$$

where $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$ are functions to be determined, and which are dimensionless. This form for $\hat{A}(\omega)$ is then substituted into Eq. (21) and the commutator evaluated using the quasimode form, Eq. (13), for $\hat{H}_F$ and the commutation

rules in Eq. (14). The coefficients of the the operators $\hat{a}_i$ and $\hat{b}(\Delta)$ on both sides of Eq. (21) are then equated, giving a set of coupled equations for the $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$. These are

$$(\omega_i-\omega)\alpha_i(\omega)+\sum_{j\neq i} v_{ji}\alpha_j(\omega) + \int d\Delta\, \rho_c(\Delta)\beta(\omega,\Delta)W_i^*(\Delta)=0, \quad (23)$$

$$(\Delta-\omega)\beta(\omega,\Delta)+\sum_i W_i(\Delta)\alpha_i(\omega)=0. \quad (24)$$

To solve Eqs.(23) and (24) for the unknown $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$, we first solve for β in terms of the α_i. This gives

$$\beta(\omega,\Delta)=\left[\mathrm{P}\frac{1}{\omega-\Delta}+z(\omega)\delta(\omega-\Delta)\right]\sum_j W_j(\Delta)\alpha_j(\omega), \quad (25)$$

where $z(\omega)$ is a dimensionless function yet to be determined. This expression is then substituted into Eq. (23) to obtain a set of linear homogeneous equations for the $\alpha_i(\omega)$ in the form

$$(\omega_i-\omega)\alpha_i(\omega)+\sum_{j\neq i} v_{ji}\alpha_j(\omega)+\sum_j F_{ij}\alpha_j(\omega) + \sum_j W_i^*(\omega)W_j(\omega)\rho_c(\omega)z(\omega)\alpha_j(\omega)=0. \quad (26)$$

In these equations, a frequency shift matrix $F_{ij}(\omega)$ appears, which involves a principal integral of products of the discrete-continuum quasimode coupling constants together with the quasicontinuum mode density. This is defined by

$$F_{ij}(\omega)=\mathrm{P}\int d\Delta\, \rho_c(\Delta)\frac{W_i^*(\Delta)W_j(\Delta)}{\omega-\Delta} \quad (27)$$

and satisfies the Hermiticity condition $F_{ji}=F_{ij}^*$.

Equation (26) can be written in the matrix form

$$\mathbf{m}\boldsymbol{\alpha}=0, \quad (28)$$

where the column matrix $\boldsymbol{\alpha}\equiv\{\alpha_1(\omega),\alpha_2(\omega),\alpha_3(\omega),\ldots\}^\top$ and the square matrix $\mathbf{m}$ is given by

$$\mathbf{m}_{ij}(\omega)=(\omega_i-\omega)\delta_{ij}+(1-\delta_{ij})v_{ji}+F_{ij}(\omega) + W_i^*(\omega)W_j(\omega)\rho_c(\omega)z(\omega). \quad (29)$$

2. Solution of equations for amplitudes $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$

The approach used to solve these equations is as follows. It is clear that Eq. (28) can give an (unnormalized) solution for $\boldsymbol{\alpha}$ in terms of the function $\rho_c(\omega)z(\omega)$. We can now use Eq. (28) itself to obtain the expression for $\rho_c(\omega)z(\omega)$, subject to the assumption that the quantity $\Sigma_i W_i(\omega)\alpha_i(\omega)$ is nonzero. This assumption will be verified *a posteriori* from the normalization condition for the $\alpha_i(\omega)$, which will follow (see below) from the requirement that the form for the $\hat{A}(\omega)$ given in Eq. (22) satisfies the commutator relation $[\hat{A}(\omega),\hat{A}^\dagger(\omega')]=\delta(\omega-\omega')/\rho(\omega)$ [Eq. (17)]. This indeed leads to a nonzero expression for $\Sigma_i W_i(\omega)\alpha_i(\omega)$ [see Eq. (39) below]. After finding both $\rho_c(\omega)z(\omega)$ and $\Sigma_i W_i(\omega)\alpha_i(\omega)$, the results can be substituted back into Eqs. (26). By eliminating the factor $\Sigma_i W_i(\omega)\alpha_i(\omega)$ from the last term in Eqs. (26), we obtain a set of inhomogeneous linear equations for the $\alpha_i(\omega)$, which can then be solved for the $\alpha_i(\omega)$ [and hence $\beta(\omega,\Delta)$].

The general expression for $\rho_c(\omega)\ z(\omega)$ can be obtained from the matrix equation (28). With $\mathbf{E}$ the unit matrix we introduce the square matrix $\boldsymbol{\Omega}$, the column matrix $\mathbf{W}^*$, and the row matrix $\mathbf{W}^T$ by

$$\boldsymbol{\Omega}_{ij}(\omega)=\omega_i\delta_{ij}+(1-\delta_{ij})v_{ji}+F_{ij}(\omega) \quad (30)$$

and $\mathbf{W}^*(\omega)\equiv\{W_1^*(\omega),W_2^*(\omega),W_3^*(\omega),\ldots\}^\top$, $\mathbf{W}^T(\omega)\equiv\{W_1(\omega),W_2(\omega),W_3(\omega),\ldots\}$, and then write Eq. (28) in the form

$$[-(\omega\mathbf{E}-\boldsymbol{\Omega})+\rho_c(\omega)z(\omega)\mathbf{W}^*\mathbf{W}^T]\boldsymbol{\alpha}=0. \quad (31)$$

Now the matrix $\boldsymbol{\Omega}$ is Hermitian and positive definite, having real eigenvalues close to the real and positive ω_i. The matrix $\omega\mathbf{E}-\boldsymbol{\Omega}$ can be hence assumed to be invertible, so by multiplying Eq. (31) from the left by $\mathbf{W}^T(\omega\mathbf{E}-\boldsymbol{\Omega})^{-1}$ we see that

$$[-1+\rho_c(\omega)z(\omega)J(\omega)]\mathbf{W}^T\boldsymbol{\alpha}=0, \quad (32)$$

where the function $J(\omega)$ is defined by

$$J(\omega)=\mathbf{W}^T(\omega\mathbf{E}-\boldsymbol{\Omega})^{-1}\mathbf{W}^*. \quad (33)$$

Now the quantity $\mathbf{W}^T\boldsymbol{\alpha}$ is equal to $\Sigma_i W_i(\omega)\alpha_i(\omega)$, which is assumed to be nonzero for reasons explained above. This means that $[-1+\rho_c(\omega)z(\omega)J(\omega)]=0$, and this gives for $\rho_c(\omega)z(\omega)$ the general result:

$$\rho_c(\omega)z(\omega)=\left\{\sum_{ij} W_i(\omega)(\omega\mathbf{E}-\boldsymbol{\Omega}(\omega))_{ij}^{-1}W_j^*(\omega)\right\}^{-1}, \quad (34)$$

which only involves the various coupling constants and angular frequencies, along with the quasicontinuum mode density. In general the ω dependence of the result for $\rho_c(\omega)z(\omega)$ is complicated, since both the coupling constants W_i and the matrix $\boldsymbol{\Omega}$ (by the matrix F) will depend on ω. In some important cases however, their ω dependence can be ignored.

As indicated previously, Eqs. (26) or (28) only determine the $\alpha_i(\omega)$ [and hence $\beta(\omega,\Delta)$] to within an arbitary scaling factor, as can be seen from their linear form. The normalization of the solutions is fixed by noting that we need $\hat{A}(\omega)$, Eq. (22), to satisfy the commutator relation $[\hat{A}(\omega),\hat{A}^\dagger(\omega')]=\delta(\omega-\omega')/\rho(\omega)$ [Eq.(17)]. This leads to the condition

$$\sum \alpha_i(\omega)\alpha_i^*(\omega') + \int d\Delta\, \rho_c(\Delta)\beta(\omega,\Delta)\beta^*(\omega',\Delta) = \delta(\omega-\omega')/\rho(\omega). \tag{35}$$

Then substituting for $\beta(\omega,\Delta)$ from Eq. (25) and using Eq. (27), we find after considerable algebra that

$$\begin{aligned}\sum \alpha_i(\omega)\alpha_i^*(\omega') &+ \delta(\omega-\omega')(\pi^2+|z(\omega)|^2)\rho_c(\omega)\\ &\times\sum_{ij} W_i(\omega)W_j^*(\omega)\alpha_i(\omega)\alpha_j^*(\omega)\\ &+ \mathrm{P}\frac{1}{\omega-\omega'}\sum_{ij}\alpha_i(\omega)\alpha_j^*(\omega')[F_{ij}^*(\omega')\\ &- F_{ji}(\omega) + z^*(\omega')\rho_c(\omega')W_i(\omega')W_j^*(\omega')\\ &- z(\omega)\rho_c(\omega)W_i(\omega)W_j^*(\omega)]\\ &= \delta(\omega-\omega')/\rho(\omega).\end{aligned} \tag{36}$$

Note that we have used certain properties of the principal parts and delta functions (see, for example, Ref. [12])

$$\begin{aligned}\delta(\omega-\Delta)\,\delta(\omega'-\Delta) &= \delta(\omega-\omega')\,\delta(\omega-\Delta)\\ &= \delta(\omega-\omega')\,\delta(\omega'-\Delta),\end{aligned}$$

$$\mathrm{P}\frac{1}{\omega'-\Delta}\delta(\omega-\Delta) = \mathrm{P}\frac{1}{\omega'-\omega}\delta(\omega-\Delta)$$

$$\mathrm{P}\frac{1}{\omega-\Delta}\mathrm{P}\frac{1}{\omega'-\Delta} = \mathrm{P}\frac{1}{\omega-\omega'}\left(\mathrm{P}\frac{1}{\omega'-\Delta}-\mathrm{P}\frac{1}{\omega-\Delta}\right) + \pi^2\delta(\omega-\Delta)\,\delta(\omega'-\Delta) \tag{37}$$

to obtain the last equation. We then also use

$$\mathrm{P}\frac{1}{\omega-\omega'}(\omega-\omega') = 1 \tag{38}$$

along with Eq. (26) to substitute for $\Sigma_j F_{ij}^*(\omega')\alpha_j^*(\omega')$ and $\Sigma_i F_{ji}(\omega)\alpha_i(\omega)$ and finally obtain

$$\begin{aligned}\sum_{ij} W_i(\omega)W_j^*(\omega)\alpha_i(\omega)\alpha_j^*(\omega) &= \left|\sum_i W_i(\omega)\alpha_i(\omega)\right|^2\\ &= \frac{1}{\rho(\omega)\rho_c(\omega)(\pi^2+|z(\omega)|^2)}.\end{aligned} \tag{39}$$

This fixes, albeit with the coefficients $W_i(\omega)$, the normalization of the $\alpha_i(\omega)$. Note the appearance of both mode densities in the result. Finally, with a suitable choice of the overall phase we can fix the result for the important quantity $\Sigma_i W_i(\omega)\alpha_i(\omega)$ to be

$$\sum_i W_i(\omega)\alpha_i(\omega) = \frac{1}{\sqrt{\rho(\omega)\rho_c(\omega)}[\pi+iz(\omega)]}. \tag{40}$$

Having obtained this result for $\Sigma_i W_i(\omega)\alpha_i(\omega)$ we then substitute back into Eqs. (26), eliminating this factor from the last term to give a set of inhomogeneous linear equations for the $\alpha_i(\omega)$:

$$\begin{aligned}(\omega-\omega_i)\alpha_i(\omega) - \sum_{j\neq i} v_{ji}\alpha_j(\omega) - \sum_j F_{ij}\alpha_j(\omega)\\ = \frac{W_i^*(\omega)\rho_c(\omega)z(\omega)}{\sqrt{\rho(\omega)\rho_c(\omega)}[\pi+iz(\omega)]}.\end{aligned} \tag{41}$$

After some algebra, introducing the matrix $\mathbf{\Omega}(\omega)$ from Eq. (30) and then substituting from Eq. (34) for $[\rho_c(\omega)z(\omega)]^{-1}$, the last equations can be solved for the $\alpha_i(\omega)$, giving the solution in matrix form as

$$\boldsymbol{\alpha}(\omega) = -i\sqrt{\frac{\rho_c(\omega)}{\rho(\omega)}}\frac{1}{[1-i\pi\rho_c(\omega)\mathbf{W}^T(\omega)(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{-1}\mathbf{W}^*(\omega)]}(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{-1}\mathbf{W}^*(\omega). \tag{42}$$

In this result all the terms that in general depend on ω are explicitly identified. It is also convenient to write the inverse matrix in terms of its determinant and the adjugate matrix by

$$(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{-1} = (\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{ADJ}/|\omega\mathbf{E}-\mathbf{\Omega}(\omega)| \tag{43}$$

and then the solution for $\boldsymbol{\alpha}(\omega)$ becomes

$$\boldsymbol{\alpha}(\omega) = -i\sqrt{\frac{\rho_c(\omega)}{\rho(\omega)}}\frac{1}{[|\omega\mathbf{E}-\mathbf{\Omega}(\omega)|-i\pi\rho_c(\omega)\mathbf{W}^T(\omega)(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{ADJ}\mathbf{W}^*(\omega)]}(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{ADJ}\mathbf{W}^*(\omega). \tag{44}$$

The result for the expansion coefficient $\beta(\omega,\Delta)$ then follows from Eq. (25) and substituting for $\rho_c(\omega)z(\omega)$ from Eq. (34). After some algebra we find that

$$\beta(\omega,\Delta)=-i\frac{1}{\sqrt{\rho(\omega)\rho_c(\omega)}}\frac{\left[\delta(\omega-\Delta)+\mathrm{P}\,\frac{1}{\omega-\Delta}\rho_c(\omega)\mathbf{W}^T(\omega)(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{-1}\mathbf{W}^*(\omega)\right]}{[1-i\pi\rho_c(\omega)\mathbf{W}^T(\omega)(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{-1}\mathbf{W}^*(\omega)]}. \tag{45}$$

We see that the solutions for the $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$ only involve the various coupling constants and the mode densities.

3. Coupling constants and reservoir structure function

Introducing the column matrix $\boldsymbol{\lambda}_k\equiv\{\lambda_{k1},\lambda_{k2},\lambda_{k3},\ldots\}^\top$ the expression (19) for the coupling constant $g^k(\omega)$ can be written as

$$g^k(\omega)=-i\sqrt{\frac{\rho_c(\omega)}{\rho(\omega)}}\frac{1}{[|\omega\mathbf{E}-\mathbf{\Omega}(\omega)|-i\pi\rho_c(\omega)\mathbf{W}^T(\omega)(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{ADJ}\mathbf{W}^*(\omega)]}\boldsymbol{\lambda}_k^T(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{ADJ}\mathbf{W}^*(\omega) \tag{46}$$

$$=-i\sqrt{\frac{\rho_c(\omega)}{\rho(\omega)}}\frac{Q_{n-1}^k(\omega)}{P_n(\omega)}, \tag{47}$$

where the functions $P_n(\omega)$ and $Q_{n-1}^k(\omega)$ are defined by

$$\begin{aligned}P_n(\omega)&=|\omega\mathbf{E}-\mathbf{\Omega}(\omega)|-i\pi\rho_c(\omega)\\&\quad\times\mathbf{W}^T(\omega)(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{ADJ}\mathbf{W}^*(\omega)\\&=|\omega\mathbf{E}-\mathbf{\Omega}(\omega)|-i\pi\rho_c(\omega)\\&\quad\times\sum_{ij}W_i(\omega)(\omega\mathbf{E}-\mathbf{\Omega}(\omega))_{ij}^{ADJ}W_j^*(\omega)\end{aligned} \tag{48}$$

$$\begin{aligned}Q_{n-1}^k(\omega)&=\boldsymbol{\lambda}_k^T(\omega\mathbf{E}-\mathbf{\Omega}(\omega))^{ADJ}\mathbf{W}^*(\omega)\\&=\sum_{ij}\lambda_{ki}(\omega\mathbf{E}-\mathbf{\Omega}(\omega))_{ij}^{ADJ}W_j^*(\omega).\end{aligned} \tag{49}$$

In the case where the ω dependence of the quantities $\rho_c(\omega)$, $F_{ij}(\omega)$, and $W_i(\omega)$ can be ignored, $P_n(\omega)$ and $Q_{n-1}(\omega)$ would be polynomials in ω of degrees n and $n-1$, respectively, as will be seen in Sec. IV.

The reservoir structure function can then be expressed as $(C=1)$:

$$D^k(\omega)=\rho_c(\omega)\frac{|Q_{n-1}^k(\omega)|^2}{|P_n(\omega)|^2}, \tag{50}$$

where we note the cancellation of the true mode density $\rho(\omega)$ and the proportionality to the quasicontinuum mode density $\rho_c(\omega)$. The significance of the $\rho(\omega)$ cancellation will be discussed in Sec. III C. There is, however, further dependence on the quasicontinuum mode density within the function $P_n(\omega)$, as can be seen from Eq. (48). The role of this dependence will be discussed in Sec. IV when we have obtained expressions for the reservoir structure function for specific cases.

In summary, if we are given the Hamiltonian in the quasimode form, Eq. (13), we can obtain the true mode operators (22) which satisfy the eigenoperator condition Eq. (21). The coefficients $\alpha_i(\omega)$ are found by solving $\mathbf{m}\boldsymbol{\alpha}=0$, Eq. (28); the function $z(\omega)$ occurring in $\mathbf{m}$ is obtained from Eq. (28) and given by Eq. (34). The solutions for $\alpha_i(\omega)$ are scaled in accordance with Eq. (35) and the normalization for the quantity $\Sigma_i W_i(\omega)\alpha_i(\omega)$ is given in Eqs. (39) and (40). The normalized solutions for $\alpha_i(\omega)$ are obtained as Eqs. (42) or (44). The coefficients $\beta(\omega,\Delta)$ are then found from Eq. (25) and the result is given in Eq. (45). The true mode coupling constant $g^k(\omega)$ and the reservoir structure function $D^k(\omega)$ are obtained as Eqs. (47) and (50). These results involve the functions $P_n(\omega)$ and $Q_{n-1}^k(\omega)$ defined in Eqs. (48) and (49). The results depend on the quasicontinuum mode density ρ_c as well as on the various coupling constants and angular frequencies. It should be noted that a unique expression has been obtained for $z(\omega)$, and hence for the $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$, even though the determinental equation $|\mathbf{m}|=0$ might appear to give anything up to n solutions, where n is the number of discrete quasimodes. This feature is due to the specific form of the matrix $\mathbf{m}$ that is involved. The overall process amounts to a *diagonalization* because the EM field Hamiltonian in the nondiagonal quasimode form, is now replaced by the diagonal true mode form given by Eq. (16).

C. Inverse diagonalization: Undressing the true mode operators

We can also proceed in the opposite direction from Fano diagonalization, that is, we can also find the quasimode operators $\hat{a}_i$ and $\hat{b}(\Delta)$ in terms of the true mode operators $\hat{A}(\omega)$. In general [68,67] the quasimode annihilation operators $\hat{a}_i$ and $\hat{b}(\Delta)$ can also be expressed as linear combinations of the true mode annihilation operators $\hat{A}(\omega)$ in the form

$$\hat{a}_i=\int d\omega\,\rho(\omega)\gamma_i(\omega)\hat{A}(\omega),$$

$$\hat{b}(\Delta)=\int d\omega\,\rho(\omega)\delta(\Delta,\omega)\hat{A}(\omega), \tag{51}$$

where the functions $\gamma_i(\omega)$ and $\delta(\Delta,\omega)$ have to be determined. These can be obtained in terms of the $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$ by evaluating the commutators $[\hat{A}(\omega),\hat{a}_i^\dagger]$ and $[\hat{A}(\omega),\hat{b}(\Delta)^\dagger]$ using the basic commutation rules in Eqs.(17) and (14). For the first commutator, on substituting for $\hat{A}(\omega)$ from Eq. (22) we obtain $\alpha_i(\omega)$, on the other hand, substituting instead for $\hat{a}_i$ from Eq. (51) gives $\gamma_i^*(\omega)$, and hence $\alpha_i=\gamma_i^*$. Carrying out a similar process for the second commutator gives the result $\beta=\delta^*$ and thus

$$\hat{a}_i=\int d\omega\,\rho(\omega)\alpha_i^*(\omega)\hat{A}(\omega),$$

$$\hat{b}(\Delta)=\int d\omega\,\rho(\omega)\beta^*(\Delta,\omega)\hat{A}(\omega). \tag{52}$$

As has been already described in Sec. III A, the first of these two equations enables us to relate the two descriptions of the atom-field interaction given in Eqs. (15) and (18). Ultimately, the key expression we have obtained in Eq. (19) for the atom-true mode coupling constant rests on this result. As we will see in Sec. IV, this enables us to relate pseudomodes to the discrete quasimodes.

As a final check of the detailed expressions, in Appendix C we start with the field Hamiltonian in the quasimode form, Eq. (13), then substitute our solutions for $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$ into the expressions for $\hat{a}_i$ and $\hat{b}(\Delta)$ given in Eqs. (52). On evaluating the result, the Hamiltonian in the true mode form, Eq. (16), is obtained—as required for consistency.

It has already been noted in Sec. III B that the final expression for the reservoir structure function $D^k(\omega)$ in terms of quasimode quantities is independent of the true mode density $\rho(\omega)$. Also, we have found no equation that actually gives an expression for $\rho(\omega)$ in terms of the quasimode quantities, including the continuum quasimode density $\rho_c(\Delta)$—a somewhat surprising result. The true mode density therefore does not play an important role in the quasimode theory. The reason for this is not that hard to find, however. The theory can be recast with *both* the $\rho(\omega)$ and $\rho_c(\Delta)$ factors incorporated into the various operators and coupling constants. In Appendix B we show that $\rho(\omega)$ and $\rho_c(\Delta)$ can be scaled away to unity. For example, from Eqs.(42), (45), and (22) we see that the true mode annihilation operator is proportional to $1/\sqrt{\rho(\omega)}$, the other (operator) factor only depending on quasimode quantities. Hence (as in Appendix B) we may scale away the $\rho(\omega)$ dependence via the substitution:

$$\hat{A}(\omega)=\frac{\hat{A}^{(s)}(\omega)}{\sqrt{\rho(\omega)}}, \tag{53}$$

where $\hat{A}^{(s)}(\omega)$ is independent of ρ. If this substitution is made, then the field Hamiltonian is given by

$$\hat{H}_F=\int d\omega\,\hbar\omega\hat{A}^{(s)\dagger}(\omega)\hat{A}^{(s)}(\omega) \tag{54}$$

without any $\rho(\omega)$ term.

IV. APPLICATIONS

A. Case of a single quasimode

For this case no coupling constant between discrete quasimodes is present and we may easily allow for a nonzero shift matrix element F_{11} and for nonconstant $W_i(\Delta)$. Noting that $[\omega\mathbf{E}-\mathbf{\Omega}(\omega)]^{ADJ}=1$ and $|\omega\mathbf{E}-\mathbf{\Omega}(\omega)|=\omega-\omega_1-F_{11}(\omega)$, a simple evaluation of Eqs. (34), (42), and (47) gives the following results:

$$\rho_c(\omega)z(\omega)=\frac{\omega-\omega_1-F_{11}(\omega)}{|W_1(\omega)|^2}, \tag{55}$$

$$\alpha_1(\omega)=-i\sqrt{\frac{\rho_c(\omega)}{\rho(\omega)}}\frac{W_1(\omega)^*}{\omega-\omega_1-F_{11}(\omega)-i\pi\rho_c(\omega)|W_1(\omega)|^2}, \tag{56}$$

$$g^k(\omega)=\lambda_{k1}\alpha_1(\omega)$$

$$=-i\sqrt{\frac{\rho_c(\omega)}{\rho(\omega)}}\frac{\lambda_{k1}W_1(\omega)^*}{\omega-\omega_1-F_{11}(\omega)-i\pi\rho_c(\omega)|W_1(\omega)|^2}.$$

In terms of a frequency shift $\Delta\omega_1$ and half-width $\Gamma/2$ defined as

$$\Delta\omega_1(\omega)=F_{11}(\omega), \tag{57}$$

$$\frac{\Gamma(\omega)}{2}=\pi\rho_c(\omega)|W_1(\omega)|^2, \tag{58}$$

the reservoir structure function [see Eq. (20)] for the situation where only a single atomic transition k is involved, is then found to be $(C=1)$

$$D^k(\omega)=\frac{|\lambda_{k1}|^2\Gamma(\omega)/2\pi}{[\omega-\omega_1-\Delta\omega_1(\omega)]^2+\Gamma(\omega)^2/4}. \tag{59}$$

In the situation where the quasimode density $\rho_c(\Delta)$ and the coupling constant $W_1(\Delta)$ are slowly varying functions of Δ, these quantities can be approximated as constants in the expressions for the frequency shift and width. The reservoir structure function is then a Lorentzian shape with a single pole in the lower-half plane at $\omega_1+\Delta\omega_1-i\Gamma/2$ corresponding to a single pseudomode. Thus the single discrete quasimode is associated with a single pseudomode, whose position z_1 is given by $\omega_1+\Delta\omega_1-i\Gamma/2$ in terms of quasimode quantities.

B. Case of zero discrete quasimode-quasimode coupling and flat reservoir coupling constants

The theory becomes rather simpler if there is no coupling between the discrete quasimodes, that is

$$v_{ij}\Rightarrow 0. \tag{60}$$

This could be in fact arranged by prediagonalizing the part of the Hamiltonian $\hat{H}_F$ that only involves the discrete quasimode operators. Thus we write

$$\sum_i \hbar\omega_i \hat{a}_i^\dagger \hat{a}_i + \sum_{i\neq j} \hbar v_{ij} \hat{a}_i^\dagger \hat{a}_j \tag{61}$$

in the form

$$\sum_i \hbar\xi_i \hat{c}_i^\dagger \hat{c}_i \tag{62}$$

via the transformation

$$\hat{c}_i = \sum_j U_{ij} \hat{a}_j , \tag{63}$$

where U is unitary. The last equation can be inverted to give the $\hat{a}_i$ in terms of the $\hat{c}_i$ and the result substituted in other parts of $\hat{H}_F$ [Eq. (13)] and $\hat{H}_{AF}$ [Eq. (15)]. The original coupling constants λ_{ki} and $W_i(\Delta)$ would be replaced by new coupling constants via suitable linear combinations involving the matrix U, and these generally would have similar properties (e.g., flatness) as the original ones.

The idea of replacing the structured reservoir of true modes by quasimodes, in which the continuum quasimodes constitute a flat reservoir, implies that the discrete-continuum quasimode coupling constants $W_i(\Delta)$ and the quasicontinuum mode density $\rho_c(\Delta)$ are slowly varying functions of Δ. This results in the shift matrix F_{ij} elements being small, so it would be appropriate to examine the case where they are ignored, that is

$$F_{ij} \Rightarrow 0 \tag{64}$$

with both ρ_c, and the W_i are assumed constant.

For the case $v_{ij}=0$, $F_{ij}=0$, $\rho_c(\Delta)=\rho_c$, and $W_i(\Delta)=W_i$ (constants) the quantities involved in the inverse of the matrix $\omega\mathbf{E}-\mathbf{\Omega}(\omega)$ are

$$|\omega\mathbf{E}-\mathbf{\Omega}(\omega)| = (\omega-\omega_1)(\omega-\omega_2)\cdots(\omega-\omega_n),$$

$$(\omega\mathbf{E}-\mathbf{\Omega}(\omega))_{ij}^{ADJ} = (\omega-\omega_1)(\omega-\omega_2)\cdots(\omega-\omega_{i-1}) \times(\omega-\omega_{i+1})\ldots(\omega-\omega_n)\delta_{ij}. \tag{65}$$

A straightforward application of Eqs. (34) and (44) leads to the simple results:

$$\rho_c z(\omega) = \left\{ \sum_i \frac{|W_i|^2}{\omega-\omega_i} \right\}^{-1}, \tag{66}$$

$$\alpha_i(\omega) = -i\sqrt{\frac{\rho_c}{\rho(\omega)}} W_i^* \frac{(\omega-\omega_1)(\omega-\omega_2)\cdots(\omega-\omega_{i-1})(\omega-\omega_{i+1})\cdots(\omega-\omega_n)}{P_n(\omega)}, \tag{67}$$

where the function $P_n(\omega)$ [which is defined in Eq. (48)], is now a polynomial of degree n, whose roots are designated as ξ_i. It is now given by

$$\begin{aligned} P_n(\omega) &= (\omega-\omega_1)(\omega-\omega_2)\cdots(\omega-\omega_n) \\ &\quad -i\pi\rho_c \sum_j |W_j|^2 (\omega-\omega_1)\cdots(\omega-\omega_{j-1}) \\ &\quad \times(\omega-\omega_{j+1})\cdots(\omega-\omega_n) \\ &= (\omega-\xi_1)(\omega-\xi_2)\cdots(\omega-\xi_n). \end{aligned} \tag{68}$$

For the true mode coupling constants $g^k(\omega)$, the general result in Eq. (47) can be applied to give

$$g^k(\omega) = -i\sqrt{\frac{\rho_c}{\rho(\omega)}} \frac{Q_{n-1}^k(\omega)}{(\omega-\xi_1)(\omega-\xi_2)\cdots(\omega-\xi_n)}, \tag{69}$$

where the function $Q_{n-1}^k(\omega)$ [which is defined in Eq. (49)] is now a polynomial of order $n-1$, whose roots are designated as θ_i. It is now given by

$$\begin{aligned} Q_{n-1}^k(\omega) &= \sum_i \lambda_{ki} W_i^* (\omega-\omega_1)(\omega-\omega_2)\cdots(\omega-\omega_{i-1}) \\ &\quad \times(\omega-\omega_{i+1})\cdots(\omega-\omega_n) \\ &= S_k(\omega-\theta_1)(\omega-\theta_2)\cdots(\omega-\theta_{n-1}), \end{aligned} \tag{70, 71}$$

where S_k is a strength factor defined as

$$S_k = \sum_i \lambda_{ki} W_i^*. \tag{72}$$

The reservoir structure function $D^k(\omega)$ [see Eq. (50)] for the k transition is then given by ($C=1$)

$$D^k(\omega) = \rho_c |S_k|^2 \frac{|(\omega-\theta_1)(\omega-\theta_2)\cdots(\omega-\theta_{n-1})|^2}{|(\omega-\xi_1)(\omega-\xi_2)\cdots(\omega-\xi_n)|^2}. \tag{73}$$

Since products of the form $(\omega-\xi)(\omega-\xi^*)$ can be written as $(\omega-\mathrm{Re}\,\xi)^2+(\mathrm{Im}\,\xi)^2$, the behavior of the reservoir structure function $D^k=\rho(\omega)|g^k(\omega)|^2$ [see Eq. (20)] as a function of ω is now seen to be determined by the product of n Lorentzian functions associated with $|P_n(\omega)|^2$ with the modulus squared of the polynomial of degree $n-1$ given by $|Q_{n-1}^k(\omega)|^2$. The quasicontinuum mode density merely provides an uninteresting multiplicative constant, except insofar as it is involved in expressions for the width and shift factors. In the case where there are n discrete quasimodes, then irrespective of the location of the roots ξ_i of the polynomial equation $P_n(\omega)=0$, the reservoir structure function $D^k(\omega)$ for a single quantum excitation has n poles in the lower-half

plane, each corresponding to either ξ_i or ξ_i^*. As there are n roots when n discrete quasimodes are present, we see that each discrete quasimode corresponds to one of the n pseudomodes, whose position z_i is equal to ξ_i or to ξ_i^*. Thus, for the case here where the coupling constants and the quasicontinuum mode density are independent of frequency, the feature that leads to a pseudomode is the presence of a discrete quasimode.

C. Case of two discrete quasimodes

The results in the previous section can be conveniently illustrated for the case of two discrete quasimodes. For simplicity we will again restrict the treatment to the situation where $v_{12}=0$, $F_{ij}=0$, $\rho_c(\Delta)=\rho_c$, and $W_i(\Delta)=W_i$ (constants), and just consider a two-level atom, so only two coupling constants λ_1,λ_2 are involved. In this case the atom-true mode coupling constant can be obtained from Eq. (69) and is

$$g(\omega)=-i\sqrt{\frac{\rho_c}{\rho(\omega)}}\frac{(\lambda_1 W_1^*+\lambda_2 W_2^*)(\omega-\omega_0)}{(\omega-\xi_1)(\omega-\xi_2)}, \tag{74}$$

where ω_0 and the roots $\xi_{1,2}$ of $P_2(\omega)=0$ are given by

$$\omega_0=\frac{\lambda_2 W_2^*}{(\lambda_1 W_1^*+\lambda_2 W_2^*)}\omega_1+\frac{\lambda_1 W_1^*}{(\lambda_1 W_1^*+\lambda_2 W_2^*)}\omega_2 \tag{75}$$

and

$$\xi_{1,2}=\frac{1}{2}\{(\omega_1+\omega_2)+i\pi\rho_c(|W_1|^2+|W_2|^2)\}\pm\frac{1}{2}\sqrt{\{(\omega_1-\omega_2)+i\pi\rho_c(|W_1|^2-|W_2|^2)\}^2-4\pi^2\rho_c^2|W_1|^2|W_2|^2}. \tag{76}$$

It will also be useful to introduce widths Γ_i defined by

$$\Gamma_i=2\pi\rho_c|W_i|^2 \tag{77}$$

and which can be later identified (see Sec. V) as the discrete quasimode decay rates [Eq. (99)]. These results will be now examined for special subcases.

1. Special subcase: Equal quasimode frequencies

In this case we choose

$$\omega_1=\omega_2=\omega_C \tag{78}$$

and find that

$$\omega_0=\omega_C,$$

$$\xi_{1,2}=\omega_C,\omega_C+i\pi\rho_c(|W_1|^2+|W_2|^2), \tag{79}$$

giving for the atom-true mode coupling constant

$$g(\omega)=-i\sqrt{\frac{\rho_c}{\rho(\omega)}}\frac{(\lambda_1 W_1^*+\lambda_2 W_2^*)}{\omega-\omega_c+i\pi\rho_c(|W_1|^2+|W_2|^2)}, \tag{80}$$

and for the reservoir structure function

$$D(\omega)=\rho_c\frac{|\lambda_1 W_1^*+\lambda_2 W_2^*|^2}{(\omega-\omega_c)^2+([\Gamma_1+\Gamma_2]/2)^2}. \tag{81}$$

This corresponds to a single pole in the lower-half plane for the reservoir structure function [see Eq. (20)] and thus only results in a *single* pseudomode, albeit for a case of *two* degenerate discrete quasimodes.

2. Special subcase: Equal quasimode reservoir coupling constants

In this case we choose

$$W_1=W_2=W \tag{82}$$

and find that

$$\omega_0=\omega_C+\Delta\omega_C,$$

$$\omega_C=\frac{1}{2}(\omega_1+\omega_2),$$

$$\Delta\omega_C=\frac{(\lambda_1-\lambda_2)}{2(\lambda_1+\lambda_2)}(\omega_2-\omega_1),$$

$$\xi_{1,2}=\frac{1}{2}(\omega_1+\omega_2)+i\pi\rho_c|W|^2$$

$$\pm\frac{1}{2}\sqrt{(\omega_1-\omega_2)^2-4\pi^2\rho_c^2|W|^4}. \tag{83}$$

Here ω_0 has been written in terms of the quasimodes center frequency ω_C and a frequency shift $\Delta\omega_C$, depending on the difference between the two atom-discrete quasimodes coupling constants λ_i and the discrete quasimodes detuning. There are now two regimes depending on the relative size of the discrete quasimodes separation $|\omega_1-\omega_2|$ compared to the square root of the quasicontinuum mode density $\sqrt{\rho_c}$ times the reservoir coupling constant W. Equivalently, the regimes depend on the relative size of the separation $|\omega_1-\omega_2|$ compared to the width factor (decay rate) $\Gamma=\Gamma_1=\Gamma_2=2\pi\rho_c|W|^2$.

a. Regime 1: Large separation $|\omega_1-\omega_2|>\Gamma$. Adopting the convention that $\omega_1<\omega_2$, we can write

$$\frac{1}{2}\sqrt{(\omega_1-\omega_2)^2-4\pi^2\rho_c^2|W|^4}=\frac{1}{2}(\omega_2-\omega_1)-\Delta\omega_R, \tag{84}$$

where $\Delta\omega_R$ is a reservoir induced frequency shift. The atom-true mode coupling constant now becomes:

$$g(\omega)=-i\sqrt{\frac{\rho_c}{\rho(\omega)}}\frac{(\lambda_1+\lambda_2)W^*(\omega-\omega_C-\Delta\omega_C)}{(\omega-\omega_2+\Delta\omega_R-i\pi\rho_c|W|^2)(\omega-\omega_1-\Delta\omega_R-i\pi\rho_c|W|^2)} \tag{85}$$

and the reservoir structure function is then

$$D(\omega)=\frac{|\lambda_1+\lambda_2|^2(\Gamma/2\pi)(\omega-\omega_C-\Delta\omega_C)^2}{[(\omega-\omega_2+\Delta\omega_R)^2+\Gamma^2/4][(\omega-\omega_1-\Delta\omega_R)^2+\Gamma^2/4]}. \tag{86}$$

The reservoir structure function D [see Eq. (86)] will be zero at the shifted center frequency $\omega_C+\Delta\omega_C$. There are two poles in the lower-half plane leading to Lorentzian factors centerd at frequencies $\omega_2-\Delta\omega_R$ and $\omega_1+\Delta\omega_R$, and which have equal widths $2\pi\rho_c|W|^2$. We note that the effect of the coupling to the reservoir is to decrease the effective discrete quasimodes separation by $2\Delta\omega_R$.

b. Regime 2: Small separation $|\omega_1-\omega_2|<\Gamma$. We now write

$$\frac{1}{2}\sqrt{4\pi^2\rho_c^2|W|^4-(\omega_1-\omega_2)^2}=\pi\rho_c|W|^2(1-\Delta f_\Gamma), \tag{87}$$

where Δf_Γ is a fractional change in width factors associated with discrete quasimode separation. The atom-true mode coupling constant now becomes

$$g(\omega)=-i\sqrt{\frac{\rho_c}{\rho(\omega)}}\frac{(\lambda_1+\lambda_2)W^*(\omega-\omega_C-\Delta\omega_C)}{\left[\omega-\omega_C-2i\pi\rho_c|W|^2\left(1-\frac{1}{2}\Delta f_\Gamma\right)\right](\omega-\omega_C-i\pi\rho_c|W|^2\Delta f_\Gamma)}, \tag{88}$$

and the reservoir structure function is

$$D(\omega)=\frac{|\lambda_1+\lambda_2|^2(\Gamma/2\pi)(\omega-\omega_C-\Delta\omega_C)^2}{\left[(\omega-\omega_C)^2+\Gamma^2\left(1-\frac{1}{2}\Delta f_\Gamma\right)^2\right]\left[(\omega-\omega_C)^2+\Gamma^2\left(\frac{1}{2}\Delta f_\Gamma\right)^2\right]}. \tag{89}$$

The reservoir structure function D [see Eq. (89)] will again be zero at the shifted center frequency $\omega_C+\Delta\omega_C$. There are two poles in the lower-half plane leading to Lorentzian factors both centerd at the same frequency ω_C, but which have unequal widths $2\pi\rho_c|W|^2(1-\frac{1}{2}\Delta f_\Gamma)$ and $\pi\rho_c|W|^2\Delta f_\Gamma$. If $\Delta f_\Gamma\ll 1$, one width is much smaller than the other.

In their work on super-radiance in a photonic band-gap material, Bay *et al.* [77] assume as a model for the mode density, a so-called Fano profile of the form

$$\rho(\omega)=\frac{f(\omega-\omega_C-q)^2}{\left[(\omega-\omega_C)^2+\left(\frac{1}{2}\kappa\right)^2\right]\left[(\omega-\omega_C)^2+\left(\frac{1}{2}\gamma\right)^2\right]} \tag{90}$$

with the two-level atom coupling constant $g(\omega)$ given by a slowly varying function proportional to $\sqrt{\omega}$. It is interesting to note that the reservoir structure function related to their theory is of the same form as that obtained here from Eq. (89) if the following identifications are made:

$$q\rightarrow-\Delta\omega_C,$$

$$\frac{1}{2}\kappa\rightarrow 2\pi\rho_c|W|^2\left(1-\frac{1}{2}\Delta f_\Gamma\right),$$

$$\frac{1}{2}\gamma\rightarrow\pi\rho_c|W|^2\Delta f_\Gamma. \tag{91}$$

For situations such as atomic systems coupled to the field in high Q cavities, the physics is different of course, with the resonant behavior in the reservoir structure function being due to the atom-true mode coupling constants rather than the reservoir mode density (which we assume is slowly varying). Nevertheless, our two discrete quasimode model—with

equal reservoir coupling constants W that are large compared to the discrete quasimodes detuning $|\omega_1-\omega_2|$—does provide an *equivalent* physical model for the photonic band-gap case that Bay *et al.* treated, the lack of which was commented on in the review by Lambropoulos *et al.* [22].

The band-gap case was also treated as a specific example by Garraway [59] in the original pseudomode theory paper. A model for the reservoir structure function was assumed in the form of a difference between two Lorentzians:

$$D(\omega)=w_1\frac{\Gamma_1}{(\omega-\omega_C)^2+\left(\frac{1}{2}\Gamma_1\right)^2}-w_2\frac{\Gamma_2}{(\omega-\omega_C)^2+\left(\frac{1}{2}\Gamma_2\right)^2}, \tag{92}$$

where the weights w_1, w_2 satisfy $w_1-w_2=1$. Again, apart from an overall proportionality constant this same form can be obtained here [see Eq. (89)] for the reservoir structure function D, if we choose the atom-discrete quasimode coupling constants λ_1, λ_2 to be equal (so that the frequency shift $\Delta\omega_C$ is zero):

$$\lambda_1=\lambda_2,$$

$$\Delta\omega_C=0, \tag{93}$$

and where the following identifications are made:

$$\frac{1}{2}\Gamma_1\rightarrow 2\pi\rho_c|W|^2\left(1-\frac{1}{2}\Delta f_\Gamma\right),$$

$$\frac{1}{2}\Gamma_2\rightarrow \pi\rho_c|W|^2\Delta f_\Gamma,$$

$$w_1\rightarrow\frac{1-\frac{1}{2}\Delta f_\Gamma}{1-\Delta f_\Gamma},$$

$$w_2\rightarrow\frac{\frac{1}{2}\Delta f_\Gamma}{1-\Delta f_\Gamma}. \tag{94}$$

As will be seen in Sec. V, the existence of unusual forms of the reservoir structure function (such as the presence of Lorentzians with negative weights) does not rule out Markovian master equations being applied to the atom-discrete quasimodes system. Thus, for the situation of a single quantum excitation, where the pseudomodes are always equivalent to discrete quasimodes, we can always obtain Markovian master equations for the pseudomode-atom system.

V. MARKOVIAN MASTER EQUATION FOR THE ATOM-DISCRETE QUASIMODES SYSTEM

A key idea for treating the behavior of a small system coupled to a structured reservoir is that although the behavior of the small system itself is non-Markovian, an enlarged system can be obtained that exhibits Markovian dynamics—and which includes the small system, whose dynamics can be obtained later. In our example of a multilevel atomic system coupled to the quantum EM field as a structured reservoir, we can proceed as follows. The overall system of the atom(s) plus quantum EM field is partitioned into a Markovian system consisting of the atom plus the discrete quasimodes and a flat reservoir consisting of the continuum quasimodes. The system Hamiltonian $\hat{H}_S$ is

$$\hat{H}_S=\sum_k \eta_k\hbar\omega_k(\hat{\sigma}_k^+\hat{\sigma}_k^- -\hat{\sigma}_k^-\hat{\sigma}_k^+)+\sum_i \hbar\omega_i\hat{a}_i^\dagger\hat{a}_i$$
$$+\sum_{i\neq j}\hbar v_{ij}\hat{a}_i^\dagger\hat{a}_j+\sum_k\sum_i(\hbar\lambda_{ki}^*\hat{a}_i\hat{\sigma}_k^+ +\text{H.c.}) \tag{95}$$

while the reservoir Hamiltonian $\hat{H}_R$ is

$$\hat{H}_R=\int d\Delta\,\rho_c(\Delta)\,\hbar\Delta\hat{b}^\dagger(\Delta)\hat{b}(\Delta) \tag{96}$$

and the system-reservoir interaction Hamiltonian $\hat{H}_{S-R}$ is

$$\hat{H}_{S-R}=\sum_i\int d\Delta\,\rho_c(\Delta)[\hbar W_i(\Delta)\hat{a}_i^\dagger\hat{b}(\Delta)+\text{H.c.}], \tag{97}$$

so that the total Hamiltonian is still equal to the sum of $\hat{H}_A$, $\hat{H}_F$, and $\hat{H}_{AF}$, given in Eqs. (12), (13), and (15). The distinction between the non-Markovian true mode treatment and the Markovian quasimode approach is depicted in Fig. 2.

It is of course the slowly varying nature of the coupling constants $W_i(\Delta)$ and the mode density $\rho_c(\Delta)$ that results in a Markovian master equation for the reduced density operator $\hat{\rho}$ of the atom-discrete quasimodes system. Rather than derive the master equation for the most general state of the reservoir, we will just consider the simplest case in which the reservoir of continuum quasimodes are all in the vacuum state. Again, the coupling constants W_i will be assumed constant so that no shift matrix F_{ij} elements are present. The master equation is derived via standard proceedures (Born and Markoff approximations) [12,20], which require the evaluation of two-time reservoir correlation functions in which the required reservoir operators are the quantities $\int d\Delta\,\rho_c(\Delta)W_i(\Delta)\hat{b}(\Delta)$ and their Hermitian adjoints. To obtain Markovian behavior, we require the quantities $\rho_c(\Delta)W_i(\Delta)W_j^*(\Delta)$ to be slowly varying with Δ, so that the reservoir correlation time τ_c [inversely proportional to the bandwidth of $\rho_c(\Delta)W_i(\Delta)W_j^*(\Delta)$] is sufficiently short that the interaction picture density operator hardly changes during τ_c.

The standard procedure then yields the master equation in the Lindblad form:

$$\frac{d\hat{\rho}}{dt}=\frac{-i}{\hbar}[\hat{H}_S,\ \hat{\rho}]+\sum_{ij}\pi\rho_c W_i W_j^*\{[\hat{a}_j,\hat{\rho}\hat{a}_i^\dagger]+[\hat{a}_j\hat{\rho},\hat{a}_i^\dagger]\}. \tag{98}$$

Direct couplings between the discrete quasimodes involving the v_{ij} are included in the system Hamiltonian $\hat{H}_S$. Radiative processes take place via the atom-discrete quasimodes interaction also included in $\hat{H}_S$, though still given as shown in Eq. (15). The loss of radiative energy to the reservoir is described via the relaxation terms in the master equation. The diagonal terms where $i=j$ describe the relaxation of the ith quasimode in which the decay rate is proportional to $\rho_c|W_i|^2$. A typical decay rate Γ_i for the ith discrete quasimode into the reservoir of continuum quasimodes will be

$$\Gamma_i = 2\pi\rho_c|W_i|^2. \tag{99}$$

Note that the off-diagonal terms $i\neq j$ involve pairs of discrete quasimode operators $\hat{a}_j$ and $\hat{a}_i^\dagger$, so there is also a type of rotating-wave approximation interaction taking place via the reservoir between these discrete quasimodes, as well as via direct Hamiltonian coupling involving the v_{ij}. The standard criterion for the validity of the Born-Markoff master equation Eq. (98) is that $\Gamma\tau_c \ll 1$. Processes involving multiphoton excitation of the reservoir (such as may occur for excited multilevel atoms) can be studied using standard master equation methods, thereby enabling multiple excitation of the structured reservoir to be treated via the quasimode theory.

As indicated previously, the case of an atom driven by a single mode laser field can also be treated. Here the atomic Hamiltonian term in $\hat{H}_S$ would be replaced by the dressed atom Hamiltonian given as the sum of the atomic Hamiltonian, the Hamiltonian for the single laser mode, and the atom-laser mode coupling term. For the quasimode treatment, where the cavity mode is included explicitly and the reservoir is in the vacuum state, the reservoir correlation time would be too short for any dressed atom modifications to the relaxation rates to be present [33]. This would not necessarily be the case if a true mode approach to the structured reservoir is used [35–37].

VI. NONSLOWLY VARYING MODE DENSITIES AND/OR COUPLING CONSTANTS

The basic model treated in this paper is that of atomic systems coupled to a set of discrete quasimodes of the EM field, which are in turn coupled to a continuum set of quasimodes. Although expressions for the true mode coupling constant and the reservoir structure function have been obtained for the general case where the quasimode density ρ_c and the coupling constants W_i are not necessarily slowly varying functions of Δ [see Eqs. (47) and (50)] the usefulness of the results where this is not the case is somewhat limited. As indicated in the previous section, the master equation for the atom plus discrete quasimodes system will no longer be Markovian, so the enlargement of the system based on adding the discrete quasimodes to produce a Markovian system fails.

Also, for the nonslowly varying ρ_c or W_i case, we can no longer link each discrete quasimode to a pseudomode. This situation may be seen both from the general result for the reservoir structure function [Eq. (50)] or the specific result we have obtained for the case where there is a single discrete quasimode [Eq. (59)]. In the former case, the function $P_n(\omega)$ would not be a polynomial of degree n, and therefore could have more than n roots, leading to more pseudomodes than discrete quasimodes. In the latter case involving just one discrete quasimode, even having the mode density $\rho_c(\omega)$ [and hence $\Gamma(\omega)$] represented by a single peaked function would result in $D(\omega)$ going from a single peaked function to a triple peaked function, corresponding to three pseudomodes.

However, where ρ_c or W_i are no longer slowly varying, an examination of the underlying causes for this variation may suggest replacing the present atom plus discrete and continuum quasimode model by a more elaborate system that better represents the physics of the situation, with slowly varying parameters now involved. Fano diagonalization based on such a more elaborate model could produce the desired link up with the pseudomode approach and enable a suitable, enlarged system to be identified, which has Markovian behavior, as well as overcoming the problem of treating multiple reservoir excitations. One possible elaboration would be to add a further continuum of quasimodes that are fermionic rather than bosonic.

VII. CONCLUSIONS

The theory presented above is mainly intended to apply to the important situation where the reservoir structure is actually due to the presence of a discrete system of quasimodes that are coupled to other continuum quasimodes via slowly varying coupling constants. For example, the quantum EM field in high Q resonant cavities can be accurately described in terms of the quasimode model which has these features, the discrete quasimodes being the cavity quasimodes (linked to the cavity resonances) with which the atoms inside the cavity interact, and the continuum quasimodes being the external modes.

For this situation it has been shown that, for the present case of single quantum excitations, the pseudomode method for treating atomic systems coupled to a structured reservoir of true quantum EM field modes, can be obtained by applying the Fano diagonalization method to the field described in an equivalent way as a set of discrete quasimodes together with a set of continuum quasimodes, whose mode density is assumed to be slowly varying. The interaction between the discrete and continuum quasimodes is treated in the rotating-wave approximation assuming slowly varying coupling constants, and the atomic system is assumed to be only coupled to the discrete quasimodes. The theory includes the true and continuum quasimode densities explicitly.

Expressions for the quasimode operators $\hat{a}_i$ and $\hat{b}(\Delta)$ in terms of the true mode operators $\hat{A}(\omega)$ (and vice versa) have been found, and explicit forms for the atom-true mode coupling constants have been obtained and related to the reservoir structure function that applies in pseudomode theory. We have seen that the feature that leads to a pseudomode is the presence of a discrete quasimode. Each discrete quasi-

mode corresponds to one of the pseudomodes, whose position z_i in the lower-half complex plane is determined from the roots ξ_i of a polynomial equation depending on the parameters for the quasimode system.

Although the behavior of the atom itself is non-Markovian, an enlarged system consisting of the atom plus the discrete quasimodes coupled to a flat reservoir consisting of the continuum quasimodes, exhibits Markovian dynamics, and the master equation for this enlarged system has been obtained. Using the quasimode theory, processes involving multiphoton excitation of the structured reservoir (such as may occur for excited multilevel atoms) can now be studied using standard master equation methods applied to the atom-discrete quasimodes system. Furthermore, cases with unusual forms of the reservoir structure function for single quantum excitation (for example, containing Lorentzians with negative weights) still result in Markovian master equations. Since for single quantum excitation the pseudomodes are equivalent to discrete quasimodes, we can now always obtain Markovian master equations for pseudomode-atom systems by our approach.

Although not so useful in such cases, the present theory does lead to general expressions for the true mode coupling constant and the reservoir structure function for single quantum excitation. These expressions are still valid for the general case where the quasimode density ρ_c and the coupling constants W_i are no longer slowly varying functions of Δ. However, the master equation for the atom plus discrete quasimodes system will no longer be Markovian, so the enlargement of the system based on adding the discrete quasimodes to produce a Markovian system fails. Also, for the nonslowly varying ρ_c or W_i case, we can no longer link each discrete quasimode to a pseudomode—there may be more pseudomodes than discrete quasimodes. In such cases it would be desirable to replace the present quasimode system by a more elaborate quasimode system involving only slowly varying quantities, and which better represents the underlying physical causes of the variation in W_i and ρ_c that occurs in the present model. This may make possible an extension of the Fano diagonalization approach that still links quasimodes with pseudomodes, and results in a Markovian master equation for the enlarged atom plus quasimode system. In such an elaborated system, the disadvantage of the present pseudomode treatment in treating multiple excitations of the structured reservoir could still be removed.

The treatment has been outlined in the case of a multilevel atom coupled to a structured reservoir of quantum EM field modes, but a similar approach would apply for any fermionic system coupled to a structured reservoir of bosonic oscillators. Extensions to fermionic reservoirs should also be possible. At present the treatment is restricted to cases where threshold and band-gap effects are unimportant, but may be applicable to two-dimensional photonic band-gap materials. Further extensions of the treatment to allow for atomic systems driven by single mode external laser fields are also possible, with the original atomic system being replaced by the dressed atom.

ACKNOWLEDGMENTS

The authors are grateful to D. G. Angelakis, J. Wang, P. L. Knight, and A. Imamoglu for helpful discussions. This work was supported by the United Kingdom Engineering and Physical Sciences Research Council. S.M.B. acknowledges support from the Royal Society of Edinburgh and the Scottish Executive Education and Lifelong Learning Department.

APPENDIX A: ATOMIC HAMILTONIAN

As an example of writing the atomic Hamiltonian in the form given in Eq. (12), consider a three-level atom in a V configuration with upper states $|2\rangle,|1\rangle$ and lower state $|0\rangle$, whose energy is chosen for convenience to be zero. The atomic transition operators are $\hat{\sigma}_2^+ \equiv |2\rangle\langle 0|$ and $\hat{\sigma}_1^+ \equiv |1\rangle\langle 0|$ for the two optical transitions of frequencies ω_2 and ω_1, and $\hat{\sigma}_3^+ \equiv |2\rangle\langle 1|$ for the Zeeman transition of frequency $\omega_2 - \omega_1$.

The form given in Eq. (12) is

$$\begin{aligned}\hat{H}_A &= \eta_1 \hbar \omega_1 (\hat{\sigma}_1^+ \hat{\sigma}_1^- - \hat{\sigma}_1^- \hat{\sigma}_1^+) + \eta_2 \hbar \omega_2 (\hat{\sigma}_2^+ \hat{\sigma}_2^- - \hat{\sigma}_2^- \hat{\sigma}_2^+) \\ &\quad + \eta_3 \hbar (\omega_2 - \omega_1)(\hat{\sigma}_3^+ \hat{\sigma}_3^- - \hat{\sigma}_3^- \hat{\sigma}_3^+) \\ &= \eta_1 \hbar \omega_1 (|1\rangle\langle 1| - |0\rangle\langle 0|) + \eta_2 \hbar \omega_2 (|2\rangle\langle 2| - |0\rangle\langle 0|) \\ &\quad + \eta_3 \hbar (\omega_2 - \omega_1)(|2\rangle\langle 2| - |1\rangle\langle 1|). \end{aligned} \tag{A1}$$

This expression may also be written in the form

$$\begin{aligned}\hat{H}_A = \hbar \omega_1 |1\rangle\langle 1| + \hbar \omega_2 |2\rangle\langle 2| + \hbar \omega (|0\rangle\langle 0| \\ + |1\rangle\langle 1| + |2\rangle\langle 2|), \end{aligned} \tag{A2}$$

since by equating the coefficients of the three projection operators, we obtain a set of linear equations for the η_1, η_2, η_3, and ω, which are solvable–in fact the solutions are not even unique. These equations are

$$\begin{aligned}\eta_2 \omega_2 + \eta_3 (\omega_2 - \omega_1) &= \omega_2 + \omega, \\ \eta_1 \omega_1 - \eta_3 (\omega_2 - \omega_1) &= \omega_1 + \omega, \\ -\eta_1 \omega_1 - \eta_2 \omega_2 &= \omega. \end{aligned} \tag{A3}$$

Adding these equations and then substituting into the first two gives

$$\omega = -\frac{1}{3}(\omega_1 + \omega_2), \tag{A4}$$

$$\begin{aligned}+\eta_3 (\omega_2 - \omega_1) &= -\frac{1}{3}\omega_1 + \left(\frac{2}{3} - \eta_2\right)\omega_2, \\ -\eta_3 (\omega_2 - \omega_1) &= \left(\frac{2}{3} - \eta_1\right)\omega_1 - \frac{1}{3}\omega_2. \end{aligned} \tag{A5}$$

The last two equations do not produce a unique solution for η_1, η_2, η_3. We can arbitarily choose $\eta_3 = 0$ for the low-frequency transition, and then we find that

$$\eta_1 = \frac{1}{3} - \frac{1}{3}\frac{(\omega_2 - \omega_1)}{\omega_1},$$

$$\eta_2 = \frac{1}{3} + \frac{1}{3}\frac{(\omega_2 - \omega_1)}{\omega_2}. \tag{A6}$$

This gives $\eta_1 = \eta_2 = \frac{1}{3}$ for two degenerate optical frequency transitions.

Comparing the two expressions for $\hat{H}_A$ in Eqs. (A1) and (A2), where η_1, η_2 are given by Eq. (A6) (with η_3 set to zero) and ω by Eq. (A4), we see that Eq. (A2) gives the atomic energy apart from the constant term $-\frac{1}{3}\hbar(\omega_1 + \omega_2)$.

APPENDIX B: SCALING FOR MODE DENSITIES $\rho(\omega), \rho_c(\Delta)$ EQUAL TO UNITY

The equations presented in the first part of Sec. III are based on true and quasicontinuum mode densities that are not necessarily equal to unity. To compare our expressions with those in Ref. [12], we now set out the scalings needed for the various quantities to give the Hamiltonians equivalent to $\hat{H}_F$ and $\hat{H}_{AF}$, in either true or quasimode forms [Eqs. (16), (13), (18), and (15)] in which the mode densities ρ and ρ_c are made equal to unity. The creation and anihilation operators are no longer dimensionless, the coupling constants and angular frequencies do not have dimensions of frequency, and the expansion coefficients are not dimensionless. The scaled quantities appearing in the Hamiltonians or relationships between annihilation operators will be denoted with a superscript $^{(s)}$.

The following replacements were made to the annihilation and creation operators:

$$\sqrt{\rho_c(\Delta)}\hat{b}(\Delta) \to \hat{b}^{(s)}(\Delta), \tag{B1}$$

$$\sqrt{\rho_c(\Delta)}\hat{b}^\dagger(\Delta) \to \hat{b}^{(s)\dagger}(\Delta), \tag{B2}$$

$$\sqrt{\rho(\omega)}\hat{A}(\omega) \to \hat{A}^{(s)}(\omega), \tag{B3}$$

$$\sqrt{\rho(\omega)}\hat{A}^\dagger(\omega) \to \hat{A}^{(s)\dagger}(\omega), \tag{B4}$$

to the coupling constants

$$\sqrt{\rho_c(\Delta)}W_i(\Delta) \to W_i^{(s)}(\Delta) \tag{B5}$$

and to the expansion coefficients,

$$\sqrt{\rho(\omega)}\alpha_i(\omega) \to \alpha_i(\omega)^{(s)}, \tag{B6}$$

$$\sqrt{\rho_c(\Delta)\rho(\omega)}\beta(\omega,\Delta) \to \beta^{(s)}(\omega,\Delta) \tag{B7}$$

will give the Hamiltonians equivalent to $\hat{H}_F$ and $\hat{H}_{AF}$ in either true or quasimode forms [Eqs. (16), (13), (18), and (15)] in which the mode densities are put equal to one. In addition, the modified forms of the relationships between true and quasimode annihilation operators [Eqs. (22) and (52)] can be obtained in which ρ and ρ_c are made equal to unity, as can the revised forms of the commutation rules. The latter are

$$[\hat{b}^{(s)}(\Delta), \hat{b}^{(s)\dagger}(\Delta')] = \delta(\Delta - \Delta'), \tag{B8}$$

$$[\hat{A}^{(s)}(\omega), \hat{A}^{(s)\dagger}(\omega')] = \delta(\omega - \omega'). \tag{B9}$$

In addition, the various equations for the $F_{ij}(\omega), \alpha_i(\omega), \beta(\omega,\Delta), z(\omega), g^k(\omega)$, and $D^k(\omega)$ now apply with ρ and ρ_c put equal to unity. It should be noted that the quantities $\hat{a}_i, \omega_i, v_{ij}, \Delta, \omega$ are not replaced, nor are any of the atomic quantities $\hat{H}_A, \eta_k, \omega_k, \hat{\sigma}_k^+, \hat{\sigma}_k^-$ or λ_{ki}.

APPENDIX C: THE HAMILTONIAN H_F IN DIAGONALIZED FORM

We show by starting with the field Hamiltonian in the quasimode form Eq. (13), substituting the solutions for $\alpha_i(\omega)$ and $\beta(\omega,\Delta)$ into the expressions for $\hat{a}_i$ and $\hat{b}(\Delta)$ given in Eqs. (52) and then evaluating the result, that the Hamiltonian in the true mode form, Eq. (16), is obtained. The symmetry conditions $F_{ij} = F_{ji}^*$ and $\nu_{ij} = \nu_{ji}^*$ are used throughout.

Using the expressions for $\hat{a}_i$ and $\hat{b}(\Delta)$ given in Eqs. (52) the Hamiltonian in the quasimode form, Eq. (13), is then given by

$$\hat{H}_F = \hbar \int d\omega\, \rho(\omega) \int d\omega'\, \rho(\omega')\hat{A}^\dagger(\omega)\hat{A}(\omega')I(\omega,\omega'), \tag{C1}$$

where the function $I(\omega,\omega')$ is

$$\begin{aligned} I(\omega,\omega') = &\sum_i \omega_i \alpha_i(\omega)\alpha_i^*(\omega') \\ &+ \int d\Delta\, \rho_c(\Delta)\Delta\beta(\Delta,\omega)\beta^*(\Delta,\omega') \\ &+ \sum_{ij(i\neq j)} \nu_{ij}\alpha_i(\omega)\alpha_j^*(\omega') \\ &+ \sum_i \int d\Delta\, \rho_c(\Delta) W_i(\Delta)\alpha_i(\omega)\beta^*(\Delta,\omega') \\ &+ \sum_i \int d\Delta\, \rho_c(\Delta) W_i^*(\Delta)\alpha_i^*(\omega')\beta(\Delta,\omega). \end{aligned} \tag{C2}$$

Substituting for $\beta(\omega,\Delta)$ in terms of the $\alpha_i(\omega)$ from Eq. (25), using the expression (27) for F_{ij} and then Eq. (26) for the $\alpha_i(\omega)$, we get for certain contributions within the last two terms in Eq. (C2),

$$\int d\Delta\, \rho_c(\Delta) W_i(\Delta) \beta^*(\Delta,\omega') = -(\omega_i-\omega')\alpha_i^*(\omega') - \sum_{j(j\neq i)} \nu_{ji}^* \alpha_j^*(\omega'),$$

$$\int d\Delta\, \rho_c(\Delta) W_i^*(\Delta) \beta(\Delta,\omega) = -(\omega_i-\omega)\alpha_i(\omega) - \sum_{j(j\neq i)} \nu_{ji} \alpha_j(\omega), \quad \text{(C3)}$$

leading to

$$\sum_i \int d\Delta\, \rho_c(\Delta) W_i(\Delta) \alpha_i(\omega) \beta^*(\Delta,\omega') = -\sum_i (\omega_i-\omega')\alpha_i(\omega)\alpha_i^*(\omega') - \sum_{ij(j\neq i)} \nu_{ji}^* \alpha_i(\omega)\alpha_j^*(\omega'), \quad \text{(C4)}$$

$$\sum_i \int d\Delta\, \rho_c(\Delta) W_i^*(\Delta) \alpha_i^*(\omega') \beta(\Delta,\omega) = -\sum_i (\omega_i-\omega)\alpha_i(\omega)\alpha_i^*(\omega') - \sum_{ij(j\neq i)} \nu_{ji} \alpha_j(\omega)\alpha_i^*(\omega'). \quad \text{(C5)}$$

In the second term of Eq. (C2) substitution for $\beta(\omega,\Delta)$ and $\beta^*(\omega',\Delta)$ in terms of the $\alpha_i(\omega)$ and $\alpha_j^*(\omega')$ from Eq. (25) and then using Eqs. (37) for manipulating principal integrals and delta functions leads to

$$\begin{aligned}\int d\Delta\, \rho_c(\Delta)\Delta\beta(\Delta,\omega)\beta^*(\Delta,\omega') = \sum_{ij} \Bigg\{ \Bigg[\int d\Delta\, \rho_c(\Delta)\Delta \mathrm{P}\frac{1}{\omega'-\omega}\left(\mathrm{P}\frac{1}{\omega-\Delta} - \mathrm{P}\frac{1}{\omega'-\Delta}\right) W_i(\Delta)\alpha_i(\omega) W_j^*(\Delta)\alpha_j^*(\omega') \Bigg] \\ + \pi^2 \delta(\omega-\omega')\rho_c(\omega)\omega W_i(\omega)\alpha_i(\omega) W_j^*(\omega)\alpha_j^*(\omega) \\ + \omega' \mathrm{P}\frac{1}{\omega-\omega'}\rho_c(\omega') z^*(\omega') W_i(\omega')\alpha_i(\omega) W_j^*(\omega')\alpha_j^*(\omega') \\ + \omega \mathrm{P}\frac{1}{\omega'-\omega}\rho_c(\omega) z(\omega) W_i(\omega)\alpha_i(\omega) W_j^*(\omega)\alpha_j^*(\omega') \\ + \omega\delta(\omega-\omega')\rho_c(\omega) z(\omega) z^*(\omega) W_i(\omega)\alpha_i(\omega) W_j^*(\omega)\alpha_j^*(\omega) \Bigg\}. \end{aligned} \quad \text{(C6)}$$

Then using Eq. (38) we show that

$$\Delta\left(\mathrm{P}\frac{1}{\omega-\Delta} - \mathrm{P}\frac{1}{\omega'-\Delta}\right) = \left(\omega \mathrm{P}\frac{1}{\omega-\Delta} - \omega' \mathrm{P}\frac{1}{\omega'-\Delta}\right) \quad \text{(C7)}$$

and following the introduction of the F_{ij} from Eq. (27) we get

$$\begin{aligned}\int d\Delta\, \rho_c(\Delta)\Delta\beta(\Delta,\omega)\beta^*(\Delta,\omega') = \sum_{ij} \Bigg\{ \omega \mathrm{P}\frac{1}{\omega'-\omega} F_{ji}(\omega)\alpha_i(\omega)\alpha_j^*(\omega') - \omega' \mathrm{P}\frac{1}{\omega'-\omega} F_{ji}(\omega')\alpha_i(\omega)\alpha_j^*(\omega') \\ + \omega \mathrm{P}\frac{1}{\omega'-\omega}\rho_c(\omega) z(\omega) W_i(\omega)\alpha_i(\omega) W_j^*(\omega)\alpha_j^*(\omega') \\ - \omega' \mathrm{P}\frac{1}{\omega'-\omega}\rho_c(\omega') z^*(\omega') W_i(\omega')\alpha_i(\omega) W_j^*(\omega')\alpha_j^*(\omega') \\ + \omega\delta(\omega-\omega')\rho_c(\omega)[\pi^2 + |z(\omega)|^2] W_i(\omega)\alpha_i(\omega) W_j^*(\omega)\alpha_j^*(\omega) \Bigg\}. \end{aligned} \quad \text{(C8)}$$

The last term is just $\omega\delta(\omega-\omega')/\rho(\omega)$ by using the normalization condition Eq. (39), and the $\rho_c(\omega)$ factor cancels out. The next step is to eliminate the F_{ij} using Eq. (26) for the $\alpha_i(\omega)$ twice. After further algebra using Eq. (38), again we find that

$$\int d\Delta\rho_c(\Delta)\Delta\beta(\Delta,\omega)\beta^*(\Delta,\omega') = \omega\delta(\omega-\omega')/\rho(\omega) + \sum_i \omega_i\alpha_i(\omega)\alpha_i^*(\omega') - (\omega+\omega')\sum_i \alpha_i(\omega)\alpha_i^*(\omega') + \sum_{ij(j\neq i)} \nu_{ji}^*\alpha_i(\omega)\alpha_j^*(\omega'). \quad \text{(C9)}$$

The results in Eqs. (C9), (C4), and (C5) can be substituted back into Eq. (C2) for $I(\omega,\omega')$. It is found that there is extensive cancellation leading to the final expression

$$I(\omega,\omega') = \omega\delta(\omega-\omega')/\rho(\omega) \quad \text{(C10)}$$

and hence the Hamiltonian $\hat{H}_F$ in Eq. (C1) is now in its true mode form:

$$\hat{H}_F = \int d\omega\,\rho(\omega)\,\hbar\omega\hat{A}^\dagger(\omega)\hat{A}(\omega), \quad \text{(C11)}$$

thus showing that the true and quasimode forms of $\hat{H}_F$ are equal.

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